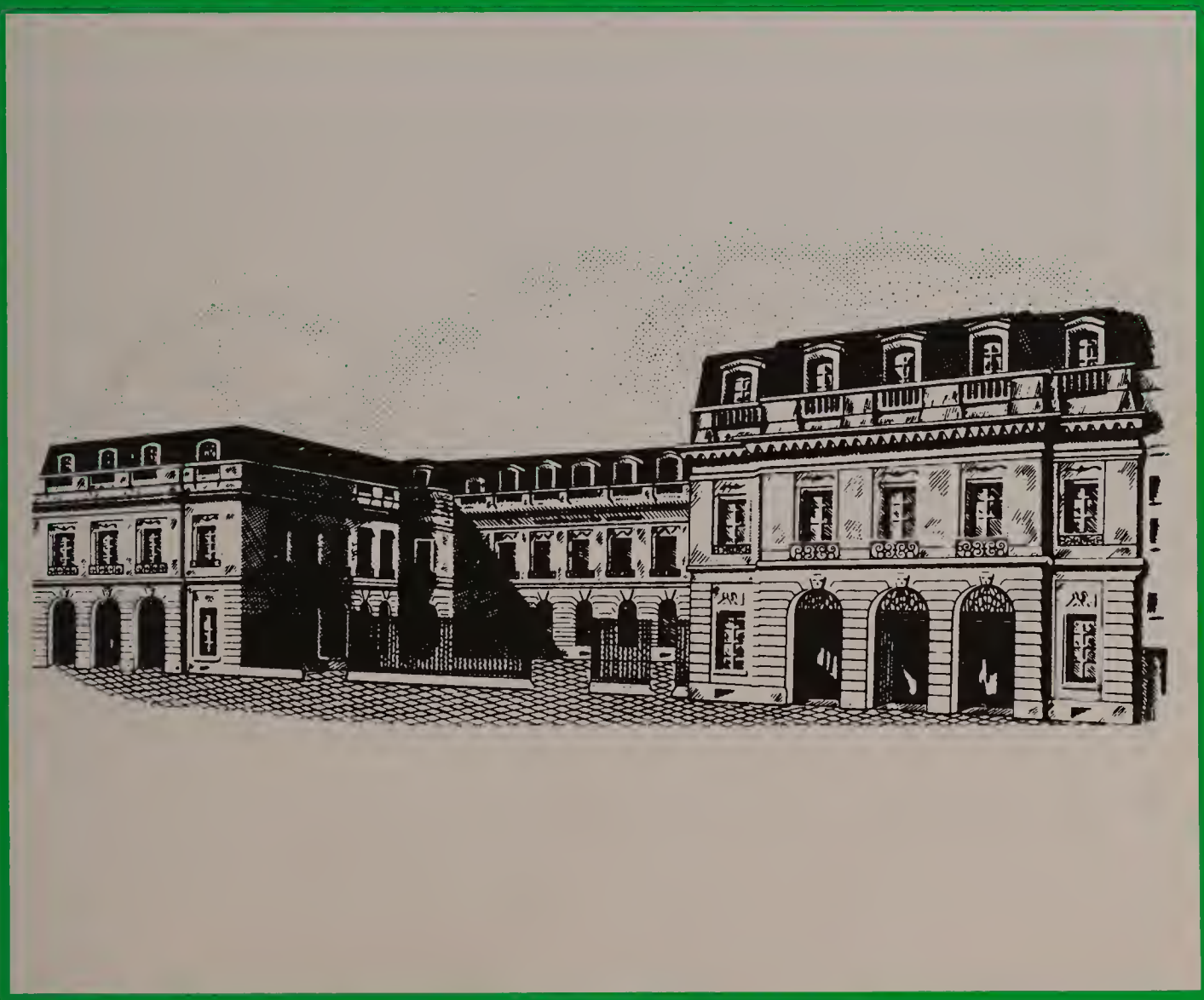
ISSN 0193-6484

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)



IUPAC

1997, Vol. 19, No. 1 (January)

Blackwell Science

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

EDITOR: Jeffrey H. Williams
SECRETARIAL ASSISTANT: Mary Patterson
PRODUCTION EDITOR: Howard Waller

All correspondence to be addressed to The Editor, Chemistry International, IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK. Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk and http://chemistry.rsc.org/rsc/iupac.htm

Editorial Advisory Board

Chairman:	E. D. BECKER	*Secretary-General*	G. SOMSEN	*Division I*
	E. BUNCEL	*CHEMRAWN Committee*	G. J. LEIGH	*Division II*
	A. SMITH	*Committee on Chemistry and Industry*	G. SAVELLI	*Division III*
	D. H. M. BOWEN	*Committee on Printed and Electronic Publications*	A. ABE	*Division IV*
			F. INGMAN	*Division V*
	I. M. MILLS	*Interdivisional Committee on Nomenclature and Symbols*	T. R. ROBERTS	*Division VI*
			(To be appointed)	*Chemistry and Human Health*
	M. E. PESTANA	*Committee on Teaching of Chemistry*		
Secretary:	J. H. WILLIAMS	*Editor*		

Subscriptions

Six issues of *Chemistry International* will be published bimonthly in 1996. The 1996 subscription rate including postage is GBP 68.50 (UK and overseas except North America) or USD 106.00 (US and Canada). The individual subscription rate is GBP 27.50 (UK and overseas except North America) or USD 39.50 (US and Canada). Microfiche subscriptions are available simultaneously with the printed edition, and microfilm at the end of the subscription year. Subscription orders may be placed directly with IUPAC's official publisher, Blackwell Science Ltd, PO Box 88, Oxford, UK; E-mail: journals.cs@blacksci.co.uk. Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Advertising. Enquiries should be sent to The Editor, Chemistry International, at the above address, or the Advertising Manager, Blackwell Science Ltd, Osney Mead, Oxford OX2 0EL, UK. Telephone: +44 (0) 1865 206206, Telex 83355 Medbok G, Fax +44 (0)1865 721205.

Despatch. The news magazine is despatched within Europe by surface mail, to other continents by various forms of air-speeded delivery: to the US* by air freight for forwarding by periodicals post, to India by air freight for guaranteeed local delivery, and to all other countries by Accelerated Surface Post.

Reproduction of Articles

Unless there is a footnote to the contrary, reproduction or translation of articles in this issue is encouraged, provided that it is accompanied by a reference to the original in *Chemistry International*. The Blackwell Science logo is a trade mark of Blackwell Science Ltd registered at the United Kingdom Trade Marks Registry.
This journal is included in the ADONIS service, whereby copies of individual articles can be printed out from compact discs (CD-ROM) on demand.

*Periodicals postage paid at Rahway, NJ. Post Master, send address changes to *Chemistry International*, c/o Mercury Airfreight International Inc., 2223 Randolf Avenue, Avenel, NJ 07001, USA.

Front cover: Maison de la Chimie, Paris, which awards a major international prize in chemistry—see page 24.

A major event for Swiss chemistry

Jacques Weber*

Geneva is going to host both the 36th IUPAC Congress and 39th IUPAC General Assembly in August 1997

The following is a slightly amended version of an article which recently appeared in *CHIMIA* (1996, Volume 50, 229–234), the official magazine of the New Swiss Chemical Society. Further information about the 36th IUPAC Congress may be found in the conference calendar section of the IUPAC Home Page http://chemistry.rsc.org/rsc/iupac.htm and on the IUPAC Congress website (http://www.unige.ch/sciences/chimie/iupac/iupac.html).

Introduction

It has already been a long story, but the event is less than one year ahead! Ever since its foundation in 1992, the Section Chemical Research (SCR) of the New Swiss Chemical Society (NSCS) had the intention of organizing in Switzerland a large event, so as to promote the image of Swiss chemistry by attracting a large number of participants to an international conference with the highest scientific level. To this end, the SCR Committee has approached several times in 1993 and 1994 Prof. Th. Kaden, the chairman of the late Swiss Committee for Chemistry, to inquire about possible opportunities in this direction. By end 1994, the SCR Committee was informed that the next free date to organize an important event such as the IUPAC Congress was 1999, as the 35th Congress was scheduled for 1995 in Istanbul and the 36th one for 1997 in Rio de Janeiro. In addition, according to a decision of the Executive Committee of IUPAC, both IUPAC Congress and General Assembly, which were organized previously every second year in different countries, should be held starting 1997 in the same country, back-to-back, with the Congress first. This automatically meant that the Swiss candidature for 1999 should be prepared in such a way as to plan the organization of both events.

Early 1995, the SCR Committee informed the NSCS Committee of the situation and of its intention to organize the IUPAC events in Switzerland, possibly in Geneva, in 1999. It immediately appeared that this organization would be such a big task (and adventure...) that the NSCS itself should be in charge of it, and not the SCR alone. In addition, after the disappearing of the Swiss Committee for Chemistry, the NSCS would be in charge of representing the community of Swiss chemists in IUPAC, and it was natural that the NSCS would act as the organizer of future IUPAC events in Switzerland. Time was short for the preparation of the Swiss candidature for 1999, and the NSCS Committee decided to proceed with a preliminary proposal to organize the events in Geneva. Consequently, the NSCS Committee asked the author of these lines to prepare the candidature files required by IUPAC for both events. This was done in March 1995, right after the visit to Geneva of several members of the Oxford IUPAC Secretariat, who found adequate both the venues chosen for the events and the conditions of accommodation. At practically the same time, the NSCS Committee appointed as follows our Organizing Committee for both IUPAC events:

Jacques Weber (chairman)—University of Geneva
Roland Darms (treasurer)—New Swiss Chemical Society
Nathalie Girard (secretary)—University of Geneva
François Diederich—Swiss Federal Institute of Technology Zürich
Thomas A. Kaden—University of Basel
Emilio Kyburz—New Swiss Chemical Society
Paul Müller—University of Geneva
Pierre Nordhoff—University of Geneva
Hans-Luzius Senti—Firmenich Geneva
Roland Wenger—Sandoz Pharma Basel
H. Michael Widmer—Ciba Basel
Alexander von Zelewsky—University of Fribourg.

In May 1995, this Organizing Committee was informed that, due to problems related to the organization of the 39th General Assembly in Rio de Janeiro in 1997, IUPAC had decided to attribute it to Geneva. The same decision was taken in July 1995 for the 36th IUPAC Congress, and both the NSCS Committee and the Organizing Committee were then faced with the unexpected task to organize the events in 1997, i.e. two years earlier than previously planned. Time was shorter than ever and, thanks to the rapid acceptation of Prof. F. Diederich to act as chairman, a Scientific Committee and an International Advisory Committee were set up as follows, their most urgent task being to prepare a

*Chairman, Organizing Committee of the 36th IUPAC Congress, Department of Physical Chemistry, University of Geneva, 30, Quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland.

Fig. 1 The large conference room (1740 seats) of the International Conference Centre of Geneva.

high-level scientific programme for the 36th IUPAC Congress:

Congress Scientific Committee

François Diederich (chairman)—Swiss Federal Institute of Technology Zürich
E. Peter Kündig—University of Geneva
Christian Leumann—University of Bern
André E. Merbach—University of Lausanne
Paul Müller—University of Geneva
Ferdinand Naef—Firmenich Geneva
Martin Quack—Swiss Federal Institute of Technology Zürich
Jacques Weber—University of Geneva
Roland Wenger—Sandoz Pharma Basel
H. Michael Widmer—Ciba Basel
Alexander von Zelewsky—University of Fribourg.

International Advisory Committee

W. Arber—Switzerland
J.-E. Bäckvall—Sweden
A. Baiker—Switzerland
D. Bellus—Switzerland
R. Breslow—USA
R.R. Ernst—Switzerland
H. Iwamura—Japan
J. Jortner—Israel
I. Karube—Japan
J.-M. Lehn—France
J. Lewis—United Kingdom
G. Modena—Italy
O.M. Nefedov—Russia
J.F. Normant—France
M.T. Reetz—Germany
J. Roeraade—Sweden
H. Rohrer—Switzerland
A. Sargeson—Australia
U.W. Suter—Switzerland
Y. Yamada—Japan

We are today about half-way on the long road of organizing these two IUPAC events, which will take place in Geneva on the following dates:

36th IUPAC Congress, 17–22 August 1997
39th IUPAC General Assembly, 23–30 August 1997.

For both events, a Professional Congress Organizer, AKM, located both in Geneva and Basle, has been selected and contracted to be in charge of a great deal of the practical organization.

It is therefore the proper time to describe here the present situation as far as the organization of both events is concerned and, in particular, to extend a warm invitation to all the members of the NSCS to participate in the 36th IUPAC Congress. Actually, the purpose of these lines is to develop somewhat the content of the First Circular of the 36th IUPAC Congress, which is just now being widely distributed among the international community of chemists, and to present the 39th General Assembly.

About IUPAC and previous IUPAC Congresses and General Assemblies

The point is not here to describe at length what IUPAC is and what are its main achievements and projects. The interested reader may consult to this end the issue 1/2 of *CHIMIA* **50** (1996), which presents (p. 38) an interview of our Swiss colleague Prof. A. Fischli, the present IUPAC president. In addition, the IUPAC Handbook 1994–1995 (Blackwell Scientific Publications, Oxford, 1994) is a must for all the curious minds in this respect. However, we found it useful to briefly summarize some relevant information about IUPAC and previous IUPAC Congresses and General Assemblies, in order to emphasize the importance for Switzerland and for Swiss chemistry of the forthcoming 1997 events.

Formed in 1919, IUPAC is a voluntary, non-governmental, non-profit association of organizations known as national adhering organizations (NAOs). An NAO represents the chemists of a member country.

IUPAC has over 40 NAOs. Twelve other countries, known as Observer Countries, are also linked to IUPAC.

IUPAC is the recognized world authority on chemical nomenclature, terminology, symbols, units, atomic weights and related topics. IUPAC provides advice on chemical matters to international agencies such as the World Health Organization (WHO), UN Food and Agricultural Organization (FAO), United Nations Education, Scientific and Cultural Organization (UNESCO), International Organization for Standardization (ISO) and Organization Internationale de Métrologie Légale (OIML).

Divisions and commissions

Some 1500 chemists throughout the world are engaged in the scientific work of IUPAC on a voluntary basis. These chemists work on IUPAC's committees and

commissions. IUPAC has 32 commissions, which are grouped into the following seven divisions:

I Physical
II Inorganic
III Organic
IV Macromolecular
V Analytical
VI Chemistry and the Environment
VII Human health

Each division has several commissions. For example, the Physical Chemistry Division has commissions on spectroscopy, electrochemistry and symbols; whilst the Applied Chemistry Division has commissions on food chemistry and atmospheric chemistry, etc. The commission members elect a division committee which regulates the affairs of the division. Commission members may be 'titular' or 'associate'. The Union makes payment towards the travel and subsistence costs of titular members, but not associate members, to attend commission meetings or general assemblies. In due course associate members frequently become titular members.

IUPAC objectives

IUPAC has four major objectives:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature; and
- to contribute to the advancement of pure and applied chemistry in all its aspects.

IUPAC Congresses

The biennial Congresses of IUPAC have been set up to constitute an outstanding forum for the presentation of modern trends and frontiers of chemical research. The first one was organized in Brussels in 1894, under the auspices of the International Association of Chemical Societies, the last ones having taken place on the following sites:

28th	Vancouver (Canada)	1981
29th	Cologne (FRG)	1983
30th	Manchester (UK)	1985
31st	Sofia (Bulgaria)	1987
32nd	Stockholm (Sweden)	1989
33rd	Budapest (Hungary)	1991
34th	Beijing (China)	1993
35th	Istanbul (Turkey)	1995

The IUPAC Congress was held once before in Switzerland (Zürich, 1955). The average attendance at these Congresses is roughly 1500 participants, with a peak of over 2000 in Stockholm.

These Congresses are in principle not financially supported by IUPAC; in addition, the organizers had until recently some freedom in defining the scope and topics of the scientific programme. However, due to the fact that the scientific programme of some of these Congresses was too broad and consequently not sufficiently focused on important specific topics, the IUPAC has recently agreed some guidelines. Namely, the IUPAC Congress should constitute a central international event in the world of chemical research, fulfilling the following goals:

1. To present the most outstanding relevant developments in modern chemistry
2. To inspire high standards of excellence in pure and applied chemistry research
3. To attract outstanding scientists to present central lectures on modern chemical research
4. To inspire the young generation of chemists in developed and developing countries.

In addition, the IUPAC recommends to launch the scientific programme for the Congress under the name *Frontiers in Chemistry*, by focusing on interdisciplinary topics. As we shall see below, the Scientific Committee of the 36th IUPAC Congress has closely followed these guidelines.

IUPAC General Assembly

The IUPAC General Assembly (GA) has little in common with a scientific conference or congress. It is indeed not open for general participation but restricted to members of IUPAC bodies that meet on this occasion. This is the case for practically all the IUPAC committees and commissions, which meet during the first half of the GA, followed by the meeting of the IUPAC Council.

The first IUPAC GA was organized in Rome in 1920, the last few having taken place on the following sites:

31st	Leuven (Belgium)	1981
32nd	Lyngby (Denmark)	1983
33rd	Lyon (France)	1985
34th	Boston (USA)	1987
35th	Lund (Sweden)	1989
36th	Hamburg (FRG)	1991
37th	Lisbon (Portugal)	1993
38th	Guilford (UK)	1995

The IUPAC GAs were held three times before in Switzerland (Lucerne/Zürich, 1936; Zürich, 1955; Davos, 1979). The average attendance at these GAs is 600–700 participants, the major problem being that the meeting of all the IUPAC bodies may require the simultaneous use of up to 50 seminar rooms on the same site!

The whole scientific programme of the GA is prepared by IUPAC itself, the local organizers being in charge of the accommodation, administrative secretariat, meeting rooms, social programme and financing.

Indeed, as far as the latter point is concerned, the rule is that the host country finances the GA, the IUPAC making a financial contribution towards the subsistence and travel expenses of its titular members.

The IUPAC events to be held in Geneva, 1997

1. 36th IUPAC Congress, Geneva, 17–22 August 1997

The general theme of the Congress, as defined by the Scientific Committee, is *Frontiers in Chemistry, New Perspectives for the 2000s*. Indeed, the aim of the organizers is to bring together distinguished experts not only to present their work but to discuss the major scientific and technological challenges facing chemistry in the next millennium.

The Scientific Committee has selected the following interdisciplinary themes that will provide a framework for lectures and discussions:

- Advanced Materials
- Catalysis and Synthetic Methods
- Molecular Properties and Reaction Pathways
- Medicinal Chemistry and Combinatorial Chemistry
- Supramolecular Chemistry and Biomolecular Recognition
- Advances in Computational Chemistry.

These themes will be presented concurrently in five parallel sessions in the traditional fields of Organic Chemistry, Inorganic Chemistry, Physical and Technical Chemistry, Analytical Chemistry and Nanosciences, Chemistry and Biology.

Each theme will be treated only in one parallel session at the same time over each day, which will allow the participants to attend all the lectures devoted to a particular theme. The conference programme will include nine plenary lectures (60 min), then, shared among the parallel sessions, 40 keynote lectures (45 min), 60 invited lectures (30 min) and 85 oral contributions (15 min). In addition, three poster sessions will be organized. The detailed programme will be presented in the Second Circular.

The list of plenary and keynote lecturers who have accepted the invitation is truly impressive and will certainly lay the foundation for a highly successful meeting, of a very high international standard, and a unique demonstration of the strength of chemical sciences, research and technology, in the broadest sense. Indeed, the following eminent scientist have accepted to present:

Plenary lectures

G. Balavoine—France
P.J. Crutzen—Germany
G. Ertl—Germany

Fig. 2 The Unil Mail building of the University of Geneva, seen from Boulevard Carl-Vogt.

O. Kahn—France
J. Nüesch—Switzerland
D. Seebach—Switzerland
P.G. Schultz—USA
C. Weissmann—Switzerland
R.N. Zare—USA

Keynote lectures

L. Addadi—Israel
J.K. Barton—USA
H.U. Blaser—Switzerland
H.-H. Brintzinger—Germany
G.R. Desiraju—India
D.A. Evans—USA
C. Floriani—Switzerland
H. Gaub—Germany
J.A. Gladysz—USA
R.H. Grubbs—USA
D. Hilvert—USA
M. Hirama—Japan
C. Khosla—USA
W. Lindner—Austria
S.J. Lippard—USA
S. Mann -United Kingdom
A. Manz—United Kingdom
B.H. Meier—Netherlands
K. Müller—Switzerland
M. Parrinello—Germany
M. Prato—Italy
K.N. Raymond—USA
J. Rebek, Jr—USA
F.E. Regnier—USA
R. Robson—Australia
J.-P. Sauvage—France
H. Schwarz—Germany
J.F. Stoddart—UK
J. Troe—Germany
M. Uhlén—Sweden
W. van Gunsteren—Switzerland
G.L. Verdine—USA
H. Waldmann—Germany
D. Wemmer—USA
A.F. Williams—Switzerland
G. Whitesides—USA
H. Yamamoto—Japan

The Congress is going to be held at the Centre International de Conférences de Genève (CICG), 15–17 Rue de Varembé, 1211 Geneva 20, which is ideally equipped with conference rooms of different sizes seating up to 1740 persons (Fig. 1). An exhibition by scientific companies (books and journals publishers, chemical instrumentation, computer hardware and software in chemistry, etc.) will also be organized at the CICG.

The registration fee for the Congress will be CHF 500

Fig. 3 The Sciences II building of the University of Geneva.

for regular participants and CHF 300 for students. It is anticipated that some bursaries will be available to help young students and Eastern Europe participants to attend the Congress. A choice of accommodation at various price categories will be available in Geneva and may be reserved at time of registration. A program for accompanying persons, together with pre- and post-conference tours will be organized.

Further information and the Second Circular, to be mailed in September 1996, may be obtained by writing to the Congress secretariat:

IUPAC '97, c/o AKM Congress Service, PO Box 37, CH—1218 LE GRAND SACONNEX, Switzerland.

The important dates to keep in mind are the following:

- 15 September 1996—Mailing Second Circular
- 28 February 1997—Submission of abstracts
- 30 April 1997—Notification of acceptance
- 15 May 1997—Deadline early registration

The Organizing Committee is convinced that it is a great honour for Switzerland to host this prestigious Congress, which probably represents one of the most important events in Swiss chemistry of the next ten years. In addition, the very high level of the scientific programme should be able to convince a great many chemists from Switzerland and abroad to participate. The organizers expect that most Swiss chemists, both from industry and academia, will attend the Congress. Students and young chemists are particularly welcome to submit an abstract, an oral contribution or a poster which would allow them to present their results to a wide international audience.

2. 39th IUPAC General Assembly, Geneva, 23–30 August 1997

The 39th IUPAC GA will be organized immediately after the Congress, in order to allow participants to attend both events. As mentioned above, a major problem for the organizers was to find a venue with 50 seminar rooms of various capacities (typically 10–30 seats). In view of this constraint, it rapidly appeared that the University of Geneva was an ideal location for the GA, specially as the modern Uni Mail Building (Fig. 2) offers very good facilities of that sort. Both Sciences II (Fig. 3) and Uni Mail buildings will therefore share the venue of the GA, with 26 meeting rooms reserved in the first facility and 24 in the second. These buildings lie quite close to one another, at a 10 min walking distance, which should not be a problem for the delegates. In addition, both buildings are modern with large open spaces, ample photocopying capacity, and availability of computer rooms and cafeterias.

Undoubtedly, though the local organizers do not have the burden of undertaking the preparation of the scientific program, the preparation of the GA is a matter of concern, as many points (maintenance of the seminar rooms, secretariat, registration desk, staff for taking care of faxes, photocopies, computers, etc.) have to be carefully considered and, for financial reasons, the involvement of AKM is smaller for the GA. However, the organizers are convinced that the competence and enthusiasm of the volunteers (students, staff of the Section of Chemistry of the University of Geneva), who have already accepted to work in the context of the GA, will allow to overcome all the difficulties and to lead to a successful 39th IUPAC General Assembly.

Conclusions

The organization of both 36th IUPAC Congress and 39th IUPAC General Assembly in Geneva represents beyond any doubt a major event for Swiss chemistry. Both the NSCS Committee and the Organizing Committee of these events expect that Swiss chemists will be enthusiastic in participating in the Congress, the high scientific level of which should have a positive impact on their education or continuous formation in chemistry. As far as sponsorship is concerned, the first responses from Swiss chemical industries and national institutions is encouraging, which shows that the importance of the events is not discussed. The organizers therefore expect to be able to present in further issues of *CHIMIA* more good news about the 1997 IUPAC events taking place in Geneva.

Consult the IUPAC Congress page on the web: http://www.unige.ch/sciences/chimie/IUPAC/IUPAC.html

Secretary General's Column

Edwin D. Becker

This is a brief report on actions by the IUPAC Bureau and the Division Presidents' plans for forthcoming activities, and developments at the Secretariat.

Future scientific policy

Possible change in the structure and function of IUPAC bodies was high on the agenda for the annual meetings of the Bureau and the Division Presidents in September, 1996. President Fischli met individually with each of the seven Division Presidents to discuss his long-range goals of making the IUPAC organization more responsive to the increasingly interdisciplinary character of chemistry and related sciences. As the diplomatic community would phrase it, there was a frank exchange of views—not always agreement on specific measures but a consensus on the need to move faster in completing important projects and in providing additional flexibility to the Divisions in responding to specific scientific problems. Meanwhile, Vice-President Jortner also met with each Division President to review his initial findings in preparation for his statutory Critical Assessment of IUPAC projects. He plans to concentrate in his assessment on broad policy and organizational aspects, rather than deal with a critique of many individual projects. I was able to participate in Prof. Jortner's meetings and found the discussions to be very helpful in learning about the vast array of activities within our Divisions and in exploring alternative organizational arrangements that can facilitate this work.

As a result of these talks and discussion at the plenary session of Division Presidents, new proposals will be drafted and considered at a special meeting of Division Presidents and Vice Presidents, along with the IUPAC Officers, to be held in Frankfurt on 24 March. At this point it is certainly not possible to forecast the detailed outcomes of this process, but I bring it up here to point out the amount of effort going into these discussions and what I perceive to be a widespread effort in the IUPAC leadership to position the Union to meet the challenges of the next decade.

Advice from outside IUPAC

In a previous column I reported that a 'brainstorming' meeting was held in June, 1996, in the USA. This meeting brought together 10 leaders from academia, government and the chemical industry in the USA and Canada to give us their frank assessment of IUPAC and to advise us on future actions. I thought that the discussions were very valuable and that the group came up with many good ideas, far too many to describe here. Overall, however, the message from this group is that despite the acknowledged continuing accomplishments of IUPAC in nomenclature and related areas and in critical evaluations of data, many leaders (especially in industry) fail to see the relevance of IUPAC to their increasingly severe requirements. This group felt that IUPAC must augment its traditional activities by undertaking projects of high visibility and recognized international importance, and our timeframe for action must be shortened to fit in with the current more hectic pace of scientific advances, both in basic research and in the chemical industry.

Edwin D. Becker, Secretary General, IUPAC

Building on this discussion, Profs Fischli and Jortner have organized a similar meeting, to take place in London on 24 February 1997, where leaders in chemistry from a number of European countries can articulate their views. In addition, a third meeting is tentatively being planned in Japan, to bring together leaders in the Southeast Asia region. Reports of these meetings will be distributed to National Adhering Organizations and will be available to the Division Presidents for their meeting in March.

Another source of advice will be the International Chemistry Council (ICC), which was recently formed by IUPAC and UNESCO (the United Nations' Educational, Scientific and Cultural Organization). The ICC was proposed by Prof. Fischli and has now been officially approved jointly by him and Mr Federico Mayor, Director General of UNESCO. The Council will hold its inaugural meeting on 31 January and is expected to provide guidance to IUPAC and UNESCO on areas of chemistry in which joint programs would be beneficial. The ICC is comprised of international leaders in chemistry and the chemical industry, including four Nobel Laureates: Dr Chris F. Garbers (South Africa), Prof. Dudley R. Herschbach (USA), Dr Yoshikazu Ito (Japan), Prof. Jean-Marie Lehn (France), Prof. Alejandro C. Paladini (Argentina), Prof. John C. Polyani (Canada), Prof. Lord Porter (UK), Prof. Hans-Jürgen Quadbeck-Seeger (Germany) and Prof. C.N. R. Rao (India).

IUPAC Congress and General Assembly

Plans for these meetings were presented to the Bureau in September, 1996, and announcements were sent to all Members of IUPAC Committees and Commissions that expect to meet at the General Assembly in Geneva, 23–30 August, 1997. I would like to use this forum to extend an invitation to all Affiliate Members to participate as observers at meetings of interest during the General Assembly. Anyone wishing to attend should contact the Secretariat as soon as possible, since arrangements must be made with appropriate Commission Chairmen.

The IUPAC Congress will be held in Geneva, 18–22 August, 1997, immediately prior to the General Assembly. A broad program of lectures in frontier areas of chemistry has been planned by the New Swiss Chemical Society, with an excellent list of speakers. Vice-President Jortner, who has been involved in developing the program, points out that 'The Union is striving toward making the biennial Congress a central event in the world of chemical research, presenting the most outstanding relevant developments in modern chemistry and inspiring high standards of excellence in pure and applied chemical research.' A new framework for the Congress, approved by Bureau (Antwerp, September, 1994), is being implemented by the organizers of the Congress in Geneva and will be fully effective in 1999 in Berlin. Further information about the 1997 IUPAC Congress can be obtained as indicated in the Conference Calendar in this issue of *Chemistry International*.

Personnel changes at the Secretariat

Two senior members of the Secretariat have recently departed. Mr P. Dass Gujral, Scientific Publications Secretary for 26 years, resigned in August, 1996. He was scheduled to retire early in 1998 but decided to leave earlier. I am sure that many readers of this column have had contacts with Dass during his long career in organizing sponsorship of IUPAC symposia and arranging publication of thousands of lectures and Commission reports, as well as a very large number of books.

Dr Jeffrey H. Williams, Deputy Executive Secretary and Information Officer, resigned in December, 1996, to become Secretary General of the European Physical Society. During the two years that Jeffrey spent with IUPAC, he has been responsible for editing *Chemistry International* and for administration of the Affiliate Membership Programme. He has been particularly successful in establishing the IUPAC Home Page on the World-Wide Web early in 1996, which has rapidly become our principal means of rapid communication with members and a source of information for the chemistry community world-wide.

Photochemistry in Italy

The European Laboratory for Non-Linear Spectroscopy (LENS) in Florence

The LENS laboratory was founded in 1991 by the Italian Ministry of University and Scientific and Technical Research. LENS is run by an International Executive Committee composed of nine members who are representatives of the Universities of Florence (Italy), Paris VI (France), Kaiserslautern (Germany), of the Max-Planck-Institut für Quantenoptik (Garching, Germany) and of the Institute for the Physics of Matter (INFM, Italy). The scientific activity of LENS is carried out under the supervision of a Scientific Committee composed of 14 members belonging to various European Laboratories.

There are 21 scientific staff in the laboratory, together with 10 technical and administrative staff members. Every year on average, 25 visitors (short and long term visits) from European and other countries are hosted by the laboratory, for research activities in collaboration with the scientific staff members or with their own projects. The funds for the research activities and the organization of the structures come from the Italian government, the European institutions (Networks, HCM, Large Scale Installation projects), and private and public industries—a total of about USD1.5 million per year. LENS has research and teaching agreements with the Chemistry and Physics Departments of the University of Florence, on the basis of which master students and PhD chemistry and physics students undertake their thesis work at LENS.

Director of LENS is *Prof. Salvatore Califano*. The facilities of the LENS are under the responsibility of *Prof. Emilio M Castellucci, Prof. Roberto Righini, Prof. Massirno Inguscio and Prof. Marcello Colocci.*

The activity of the LENS aims at:

- facilitating scientific collaboration among European researchers in the field of nonlinear laser spectroscopy and related fields;
- making available to researchers in the field the most advanced instrumentation and the necessary technical experience for its use;

- designing and realizing collaborative research projects using LENS facilities and skills;
- promoting the exchange of ideas and experience among researchers so as to facilitate the mobility of young people and to spread competencies on different European laboratories;
- collaborating and help developing of interactions with extra-European countries.

In the following we present an overview of the current and planned activities of the LENS laboratory.

Ultrafast phenomena in condensed matter (Prof. Roberto Righini)

Dynamics of different processes in condensed matter at the atomic and molecular level is investigated by means of time-resolved optical techniques.

Orientational relaxation in complex liquids

Time-resolved nonlinear spectroscopic techniques have been employed to investigate the orientational dynamics of molecules in the liquid phase. By using different laser systems, it has been possible to follow orientational relaxation over quite a large time interval, ranging from a few hundreds of femtoseconds to tens of nanoseconds. The Optical Kerr Effect and Transient Grating have been used for studying the dynamics of molecules near the disorder–order phase transition (isotropic–nematic and liquid–solid).

Evidence has been seen of the onset of a collective rotational dynamics characterized by a critical slowing down when the temperature approaches the transition point; liquid crystals such ZLI and rod-like molecules (*p*-terphenyl and *p*-quaterphenyl) have been the subjects of study. The appearance of similar collective motions has also been demonstrated in concentrated ionic solutions due to their strong inter-ionic correlations.

Time-resolved optical Kerr effect measurements in aqueous ionic solutions

Even though the aqueous state is ubiquitous, a detailed understanding of its microscopic structure remains elusive. For example, there is a paucity of experimental data concerning the electric and magnetic properties of the solvated ions which constitute the solution. This unsatisfactory state of affairs is largely a result of the lack of suitable techniques for the study of the electro-optic properties of solvated ions.

The application of an intense electromagnetic field to a fluid induces an anisotropy in its physical properties. The well-known static Kerr effect is the response of a fluid to a strong uniform static electric field. The field gives rise to differences between the components of the refractive index, parallel and perpendicular to the

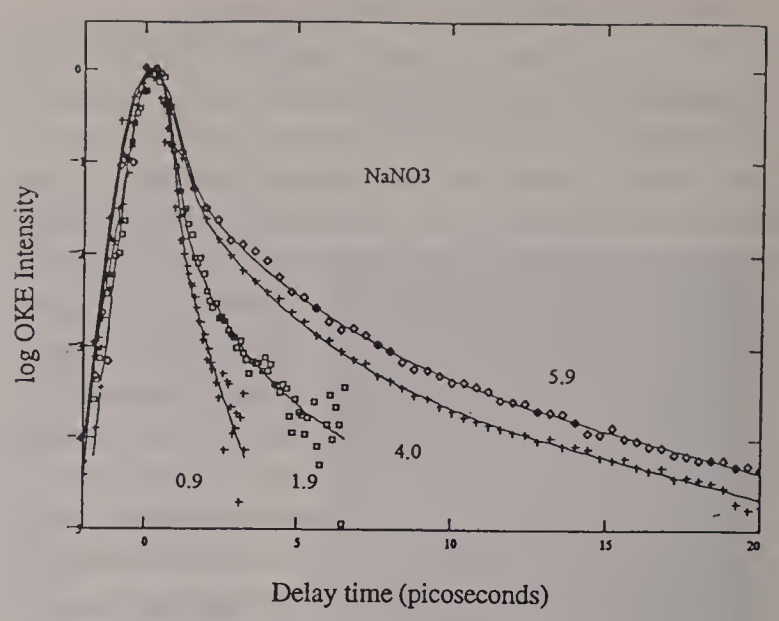


Fig. 1 Relaxation data from a femtosecond resolved optical Kerr effect measurement on aqueous solutions of sodium nitrate (concentrations are given in moles per litre).

field. Thus, a beam of linearly polarised light propagating perpendicular to the field direction and with its plane of polarization at 45° to the field becomes elliptically polarised on passage through the fluid. Physically, the molecules are being orientated by the applied electric field and the fluid is thus behaving as a uniaxial crystal, with its optic axis parallel to the field.

In the static Kerr measurement, the permanent molecular electric dipole moment makes the largest contribution to the observed induced birefringence, provided that the electric field is applied at a frequency sufficiently low as to allow the dipoles time to orientate in the applied field. However, for aqueous solutions, the static Kerr effect is a technique of limited use since ionic solutions conduct. In the optical Kerr effect (OKE), however, the applied electric field oscillates at optical frequencies and consequently the dipole contribution to the measured bulk susceptibility is lost.

Even though the OKE is now well associated with intense lasers, it was in fact predicted well before the advent of the laser. Prof. A.D. Buckingham predicted in 1956 that the oscillating electric field associated with a light beam could produce an induced birefringence in a suitably anisotropically polarizable fluid (he suggested at the time that the intense beam from a World War II search light could be focused-down to give a suitable beam).

As an example of the type of information which can be derived from OKE studies of ionic solutions, consider the nuclear contributions to the OKE of sodium nitrate and nitric acid solutions.

Figure 1 clearly demonstrates that the OKE of $NaNO_3$ solution is a strong function of solute concentration. For these solutions the anisotropic NO_3^- ion will contribute strongly to the measurements at all solute concentra-

tions, the cations being spherically symmetric and possessing an isotropic polarizability. Consequently, it is the dynamics of the nitrate ion which is the dominant contribution to the OKE of these solutions.

These OKE measurements on nitrate solutions have been interpreted as follows: besides the purely electronic response (caused by the instantaneous distortion of the ion's polarizability caused by the applied electromagnetic field—the electronic contribution to the measurement) and the fast relaxation component arising from the pure solvent, there is an intermediate concentration-independent relaxation, n(ii) ~2.2 ps, corresponding to the rotational relaxation of the NO_3^- anions, and a slow decay, whose time constant n(iii) increases with solute concentration. A similar behaviour has been observed by time-resolved OKE measurements in molten $2[Ca(NO_3)_2].3[KNO_3]$, a well known glass-forming system.

In Fig. 2 the behaviour of the two decay times corresponding to the above relaxation mechanisms, t(ii) and t(iii), in $NaNO_3$ and HNO_3 are plotted against solute concentration. The increase of n(iii) with concentration for nitric acid is clear evidence of the co-operative nature of the associated process. It is seen that the appearance of t(iii) coincides with the disappearance of 'free' water molecules, that is, when an additional solute cannot obtain a full solvation sheath due to the lack of free unassociated bulk water molecules. For concentrations above 5 M, the NO_3^- anions see each other directly, as opposed to sensing each other within a solvent sheath, thereby setting up correlated multi-ionic structures. In this sense, one may speak of the glassy or highly disordered nature of these concentrated aqueous solutions which become very viscous at these high levels of solute concentration.

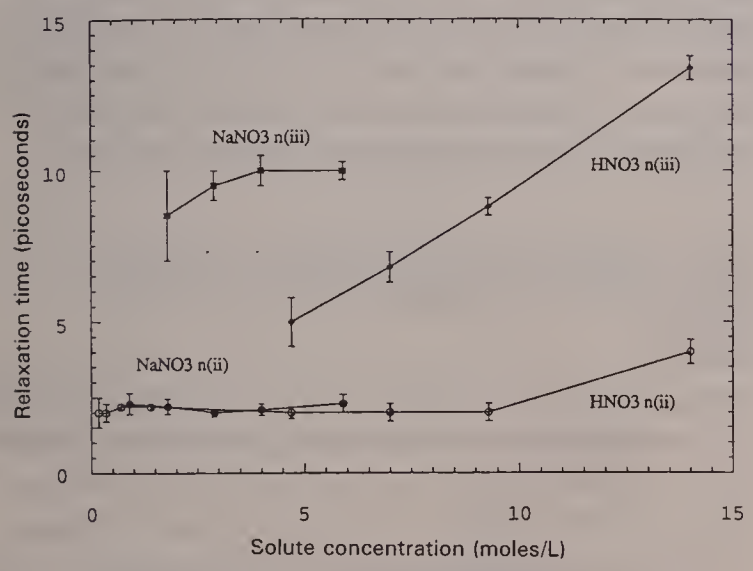


Fig. 2 Solute concentration dependence of the relaxation times derived from the data in Fig. 1. For both sets of data, n(ii) is seen to be essentially independent of solute concentration except at the highest, glass-like, concentrations; and n(iii) increases with solute concentration.

In these solutions of sodium nitrate, the concentration dependence behaviour of the nitrate anion dynamics mimics that of nitric acid, the difference between these two nitrates being that in the case of the salt the n(iii) relaxation time saturates at a relatively low solute concentration. However, we note that at these solute levels in aqueous $NaNO_3$ solution, we are not far from saturation, whereas in nitric acid we are still a little way from saturation, even at 14 M. Similarly, in these concentrated solutions where the ions will not possess complete solvation structures, that is, in this glass-like state, the sodium cations and the nitrate anions will have become 'frozen in' to a disordered system. That is, their mobility will have become somewhat reduced, the solutions are seen to be very viscous and their relaxation will become arrested as the free water molecules become involved in the strongly bound inter-ionic matrix. The protons, however, will, by virtue of their mass, be more labile in these viscous glassy solutions and will continue to move rapidly through the solution, distorting the medium as they move, giving a measurable OKE which increases with solute concentration over the range investigated in these experiments.

Energy redistribution in excited molecules

The vibrational cooling of molecules after excitation to exited electronic levels has been studied by the transient absorption technique. In the case of pyrene, the transient excited state—excited state absorption spectrum has been fully assigned, and the rate of vibrational cooling in the S_1 excited state has been shown to follow an exponential relaxation characterized by a time constant of 4 ps.

Parametric generation of ultrashort tuneable IR pulses

Tuneable ultrashort (< 150 fs) IR pulses find a very wide application in time-resolved spectroscopy. We have developed travelling wave optical parametric generators based on LBO (lithium borate) and BBO (β-barium borate) nonlinear crystals, which provide transform limited pulses operating with femtosecond and picosecond pump lasers.

Optical properties of semiconductor heterostructures (Prof. Marcello Colocci)

Research activity has mainly been devoted to the study of the optical properties of novel low-dimensioned semiconductor heterostructures. Particular attention has been paid to the possible use of such structures as novel solid-state devices.

Exciton relaxation in quantum well structures

The role that carrier thermalization carries out in exciton recombination has been carefully addressed. It has been demonstrated that excitons recombine from a thermalized distribution, even at very low lattice temperatures ($T = 2$ K), in contrast with usual assumptions. In particular, it has been found that the temperature of the carriers undergoing recombination is usually higher than the lattice temperature, except in the case of resonant excitation at the fundamental exciton transition.

These findings have a significant impact on the comprehension of exciton radiative recombination; moreover, a new interpretation of the Stokes shift effect has been proposed whereby the effect is a straightforward consequence of the thermalization hypothesis within an inhomogeneously broadened transition.

The interaction mechanisms of near-surface quantum wells with the surface states have been investigated, both in GaAs/AlGaAs and InGaAs/GaAs heterostructures. The importance of carrier tunnelling towards the surface states has been clearly evidenced. In particular, the tunnelling of isolated electrons and holes prior to exciton formation provides the main origin for the decrease of luminescence efficiency in these structures.

Finally, the effects of localization on the recombination dynamics in InGaAs/GaAs quantum wells grown on vicinal surfaces have been investigated in several samples with different Indium concentrations; an enhancement of the carrier continuum has been clearly observed as a consequence of the lateral confinement induced by strain.

Luminescence dynamics of Pb dot-like aggregates in alkali halide hosts

The optical properties of Pb^{2+} based aggregates have been studied, with particular attention devoted to the quantum-confined effects.

The scintillation features have also been investigated for possible device applications. A simple phenomenological model for the relaxation dynamics in these systems has been found to provide a nice agreement with experimental observations.

Chemical dynamics, photophysics and high resolution spectroscopy of molecules and complexes (Prof. Emilio M. Castellucci)

Vibrational relaxation mechanisms in molecular crystals were studied by means of high-resolution Raman and FT-IR techniques. The internal dynamics of molecules and van der Waals complexes in a cold molecular beam has been studied by high resolution (rovibronic) sub-Doppler spectroscopy with LIF (Laser Induced Fluorescence) and optothermal detection.

Phonon-dynamics of molecular crystals

The influence of structural disorder on vibrational relaxation in molecular crystals has been investigated by means of the high resolution Raman/Fabry–Perot tandem spectrometer developed in the laboratory.

The role of the disorder has been studied by analysing the temperature dependence of lattice and internal mode linewidths in two isomorphic benzene derivatives: the 1,4-C_6H_4BrCl (*p*-BCB) and the 1,4-$C_6H_4Br_2$ (*p*-DBB) crystals. The former shows a disorder arising from a random head-to-tail orientation of the molecular dipoles. It has been found that in *p*-BCB crystals the additional band broadening, ascribed to head-to-tail disorder, can be assumed to be temperature-independent

We have studied by high resolution Raman and FT-IR spectroscopy the vibron and phonon-bands in natural and isotopically pure ^{32}S sulphur crystals. From the spectral comparison we have assigned the bands due to the different molecules containing one or two atoms of ^{34}S, as well as one atom of ^{33}S. We have measured the bandwidth and the frequency of the vibron as a function of temperature from 10 to 140 K, both in the natural and in the isotopically pure crystal, and we have interpreted the results in terms of decay and scattering processes. In particular we have explained the nonlinear evolution of the bandwidth and of the frequency shifts with temperature in terms of scattering processes controlled by quartic terms of the anharmonic crystal potential energy.

The effect of isotopic abundance on the relaxation and dephasing mechanisms of solid chlorine was studied by looking at the line shape of the phonon-and vibron bands as a function of temperature. The Raman spectrum of natural chlorine is correctly reproduced by anharmonic lattice dynamic calculations weighted over the statistical distribution of the isotopic species.

High resolution spectroscopy and excited state dynamics in supersonic molecular beams

The high-resolution molecular beam spectrometer built in our laboratory is equipped with LIF detection, as well as with optothermal (bolometric) detection of the internal and kinetic energy content of the molecular beam. The two detection techniques are complementary. This allows us to follow, to a large extent, the fate of the energy initially deposited into the molecule (typically with a narrow bandwidth, intracavity-doubled ring dye laser), measuring both the excitation and the absorption spectrum.

Raman microscopy: applications to the studies of new materials and in studies for conservation of artistic works.

Raman microscopy is a well-established technique and is used to solve problems in diverse areas such as earth sciences, the environment, material sciences, biology, medicine, and the conservation of art.

The non-destructive identification of pigments through Raman microspectroscopy is now established at the forefront of the techniques that are available for the examination of illuminated manuscripts, paintings, books, water-colours.

The nature of the pigments on a miniature letter of illuminated medieval parchment dating from 1340 was unravelled and a confirmation of the date of preparation was given. The micro-Raman spectrometer allows the registration of the spectra of particles as small as 1 μm, with a good S/N ratio with a laser power of only some 1 μW.

Atomic and molecular physics (Prof. Massimo Inguscio)

We are exploring novel aspects in the interaction of coherent light with atoms and molecules, mostly motivated by fundamental problems in physics. Several results have been achieved which have led to a better understanding of the structure of matter

Precision atomic spectroscopy

Modern techniques of nonlinear laser spectroscopy have been applied to the atomic spectrum of helium. In particular, high resolution frequency measurements of an optical transition of this simple atom have been achieved. For this purpose, a secondary frequency standard at 778 nm has been developed by locking a semiconductor diode laser on the Doppler-free signal from a two-photon transition in rubidium.

Comparison with an accurate theoretical model has allowed the precise determination of the Lamb shift of the $^3S_1$ level. Accurate measurements of the isotope effect have lead to a determination of the nuclear radius of ^3He. Most of these results have been made possible by the investigations of the properties in the visible range of new fast detectors such as the metal-insulator-metal (MIM) point contact diode and the Schottky diode.

Spectroscopy using semiconductor diode lasers

The development of the extended cavity configuration has allowed us to perform several spectroscopic investigations with both high sensitivity and high resolution. Overtone molecular spectra in the near infrared have been investigated with a sensitivity of one part in 10^8. More recently the technique has been applied to the DFB lasers operating in the 1–2 μm region. In this case the cavity simply is extended using a mirror; laser linewidths down to 100 kHz are achieved and lower molecular overtones have been reached with an increase in sensitivity. Spectroscopic results range from a fundamental metrology of the helium resonances, where subdoppler recordings of molecular caesium have been obtained, to applied spectroscopy with the detection of ammonia.

Far infrared spectroscopy

Tuneable far infrared spectroscopy (TuFIR) has been successfully extended to the lightest polar molecule, LiH. Precise values for the rotational transition are now available for research of astrophysical interest. In addition, the physics of collisions with hydrogen and deuterium have been studied through the precise analysis of line shapes.

Important discoveries have also been made for molecules of atmospheric interest. In particular we have studied the pressure broadening with air of the hydroperoxyl radical, one of the constituents of the chemical cycle regulating the level of stratospheric ozone. Results from the investigation of far infrared transitions between fine structure levels in atomic oxygen have been compared with theoretical predictions from multielectron atomic models.

Magneto optical trap (MOT)

A magneto-optical trap has been successfully operated for caesium atoms. The usual configuration, using diode lasers as a radiation source, has been implemented with a facility for the high sensitivity detection of fluorescence, including photon-counting. Initial experimental investigations have been devoted to the study of collisional transfer between fine structure sublevels. In addition, multiple laser-beam excitation schemes have been developed for the study of two-photon and two-step transitions in the trapped atoms.

Coherent interactions within the atomic ionization continuum

In 1994, our investigation of coherent interactions within atomic ionization has proceeded with two principal aims: the fulfilment of the construction of, and the first tests of, an atomic beam device with an electron spectrometer, and the study of the effect of the alternating current (AC) Stark shift and laser bandwidth on multiphoton ionization. For the first goal we have carried out test experiments on the multiphoton ionization of xenon and sodium.

This new experimental device will allow us a better discrimination against background processes in our study of Laser Induced Continuum Structure and the study of transitions within the continuum by observations of the electron spectrum. For the second goal, we have performed accurate measurements of the AC Stark shift induced by non-resonant IR radiation and studied experimentally the lineshape for a three photon–two photon resonant ionization to put in evidence the effects of the laser bandwidth and its interplay with the power broadening. We have also studied a model of the possible effect of the continuum–continuum transition on continuum structure.

LENS is one of five European Laboratories, funded by the European Union, which offer to researchers working in the Member States of the European Union and Associated States the free use of their facilities, as well as the payment of travelling and living expenses during their visit. These five laboratories form a Large Scale facility for Laser–Matter Interactions and Non-linear Processes and for High Resolution Spectroscopy in the Time and Frequency Domain. The laboratories are:

European Laboratory for Nonlinear Spectroscopy (LENS)
Director: Prof. Salvatore Califano; Address: Largo Enrico Fermi 2, 50125 Florence, Italy.
Tel.: +39 55 2307823; Fax: +39 55 224072; E-mail: califano@generale.lens.unifi.it

Foundation for Research and Technology—Hellas (FORTH)
Director: Prof. Costas Fotakis; Address: PO Box 1527, Heraklion 711 10, Crete, Greece.
Tel.: +30 81 39 1473; Fax: +30 81 39 1318; E-mail: ulf@iesl.forth.gr

Laboratoire d'Optique Appliquée, Ecole Polytechnique (ENSTA-LOA)
Director: Prof. A. Antonetti; Address: F 91120, Palaiseau, France.
Tel.: +33 (1) 60 10 03 18; Fax: +33 (1) 69 31 02 20

Lund Laser Centre (LLC)
Director: Prof. S. Svanberg; Address: PO Box 118, S-221 00 Lund, Sweden.
Tel.: +46 46 2227650; Fax: +46 46 2224250

Max Born Institut für Nichtlineare Optik und Kurzzeitspektroskopie (MBI)
Director: Prof. Wolfgan Sander; Address: Rudower Chausee 6, PO Box 1107, Berlin, Germany.
Tel.: +49 30 63921301; Fax: +49 30 63921309, E-mail: sander@mbi.fta.berlin.de

News from the International Organization for Chemical Sciences in Development (IOCD)

Symposium and workshop on African medicinal plants

Over 90 scientists from industry and academia in 25 countries world-wide participated in the International Symposium on Chemistry, Biological and Pharmacological Properties of African Medicinal Plants held at Victoria Falls, Zimbabwe, from 25 to 28 February 1996. This meeting was convened by the IOCD Working Group on Plant Chemistry under the chairmanship of Prof. Kurt Hostettmann, Director, Institute of Pharmacognosy and Phytochemistry, University of Lausanne, Switzerland.

IOCD invited 12 distinguished scientists to speak on subjects ranging from the strategy of natural products isolation to the development of phytomedicines. The symposium concluded with a round-table discussion of problems relevant to the African situation: intellectual property rights; biodiversity; collaboration between Africans and Europeans and with Americans; phytomedicines; networks, etc. The proceedings of the symposium are to be published as a book by the University of Zimbabwe Press, Harare.

Preceding the symposium, from 22 to 24 February 1996, IOCD convened a Workshop on Bioactivity-Guided Isolation at the Department of Pharmacy, University of Zimbabwe, Harare, with 34 scientists, primarily natural products chemists from African countries. IOCD sponsored 15 of these scientists, providing them the full cost of their air fares, hotel and meals. IOCD also gratefully acknowledges additional travel grants to African scientists from the Commonwealth Foundation and the Third World Academy of Sciences. The International Program in the

Chemical Sciences (IPICS) of Sweden agreed to support the travel of African scientists in IPICS projects who wished to attend the symposium and workshop.

The workshop provided hands-on instruction in research techniques in the area of discovery of new biologically active compounds from plants. Special emphasis was put on bench-top bioassays and on separation methods (including planar chromatography, column chromatography, partition chromatography and new trends in high-pressure chromatography such as the coupling between HPLC and MS).

This was the fourth workshop organized by IOCD for natural products chemists, previous workshops having been held in Nairobi, Kenya (1990); Accra, Ghana (1992); and Montevideo, Uruguay (1994). IOCD is planning a fifth workshop, which will be a joint undertaking with the Programa Iberoamericano de Ciencia y Tecnologia para el Desarrollo (CYTED), to take place in Panama in February 1997.

International joint IOCD–ICYTED Symposium: Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas

Panama City, Panama, 23–26 February 1997
For further information, please contact:

Prof. Kurt Hostettmann, Institute of Pharmacognosy and Phytochemistry, University of Lausanne, BEP, CH-1015 Lausanne-Dorigny, Switzerland. Tel.: +41 21 6924561; Fax: +41 21 6924505; E-mail: Kurt.Hostettmarm@ipp.unil.ch

Workshop on Environmental Analytical Chemistry

IOCD and the Corporacion OIKOS, an Ecuadorian non-governmental organization, collaborated in conducting a workshop on environmental analytical chemistry from 6–10 May 1996, at the National Polytechnic University, Quito, Ecuador. The participants were 20 scientists from 12 institutions in Ecuador and one from Nicaragua. Corporacion OIKOS served as local organizer, selecting the participants, choosing the workshop site, and providing essential workshop services: simultaneous interpretation at the workshop sessions; computer work stations for all participants; audio-visual equipment for the lecturers, etc. The Joint IOCD/IUPAC Working Group on Environmental Analytical Chemistry for Developing Countries, chaired by Dr Walter R. Benson, drew up a curriculum and selected the instructors.

Workshop objective and curriculum: with the aim of updating the knowledge of the participants for monitoring environmental pollution, the workshop included the following topics:

- sampling procedures used in air, water, soils and food analyses;
- computerized programs for analytical methods for heavy metals, pesticides, toxins, PAH, chlorinated compounds, etc.
- an exchange of ideas on modern instrumentation, collaborative studies, use of EPA analytical programs, immunoassays, separation techniques, management styles for laboratories, quality assurance, and determinative procedures (atomic absorption and mass spectroscopy).

A summary of the responses by participants to a questionnaire evaluating the topics and instruction of the workshop indicated that they were highly satisfied with both aspects.

As possible follow-up activities, the participants decided upon the following:

1. A workshop for the Andean Region countries to be held in Ecuador, May 1997;

2. Possible translation into Spanish of the EPA 'Pesticides Laboratory Training Manual' for Latin American countries;

3. Organization of an Association of Chemists to create interest in environmental issues among Ecuador's chemists and to inventory analytical instruments used by laboratories in Ecuador. Corporacion OIKOS offered to assist the Association by providing a meeting place and an email infrastructure.

IOCD and South Africa's CSIR form joint mission for biodiversity exploration and conservation

The Council for Scientific and Industrial Research (CSIR) of South Africa and IOCD have formed a joint mission to prepare guidelines and funding prospects for establishing a program of biodiversity exploration and conservation in South Africa. This is the first mission by IOCD scientists within the framework of the Fund for Biodiversity Exploration and Conservation, a global agency for providing technical assistance to countries that seeks to arrest the loss of their biodiversity resources through linking biodiversity exploration with conservation, the former providing revenue as an incentive for the latter. IOCD has worked over the past two years under grants from the MacArthur Foundation, the US National Academy of Sciences and UNESCO to create this Fund.

IOCD designed the Fund to provide technical assistance primarily to developing countries, but in turning to IOCD and this Fund, South African scientists stated quite frankly that 'years of isolation from world markets and technological developments have left [us] lacking in many of the other components of a bioprospecting

programme, especially modern screening techniques and the ability to negotiate with multinational companies. [We] seek to build upon South Africa's existing capacities to the point where it can carry out bioprospecting in a systematic, comprehensive manner and therefore make optimal use of its biological resources.'

Further information about IOCD and its activities may be obtained from Dr Robert Maybury, Executive Director, IOCE

IOCD (USA Office), PO Box 8156, Falls Church, VA 22041, USA. Tel. and Fax: +1 703 845 9078. Email: iocd@igc.apc.org Home Page: http://www.iocd.unam.mx

World Science Report 1996

The World Science Report, published by the United Nations' Educational, Scientific and Cultural Organization (UNESCO), provides a global snapshot of the upheavals taking place in many countries as governments attempt to find ways to tie investment in research closer to today's economic and social goals without endangering the fundamental research that will provide tomorrow's innovation and economic success. From the collapse of the military industrial complex in Russia to the search for new industrial policies in Latin America, the reports provides a global perspective on the state of science, and on emerging trends such as the efforts world wide to tackle the ethical challenges raised by progress in biomedical research.

Here we give a summary of some of the points, of a more general interest, discussed in this report from UNESCO.

Ethics debate needed to avoid public backlash against science

Growing public distrust of science and technology risks fuelling the growth of political and religious movements whose dogma rejects modernity 'as a symbol of the perverted contemporary world'. To avoid both this prospect, and that of a public backlash against the work of researchers, a vigorous public debate on the ethical issues raised by scientific advances is urgently needed.

This is the warning made by Noëlle Lenoir—a prominent figure in the bioethics movement and a member of the French Constitutional Council—in a thought-provoking paper *The ethics of science: between humanism and modernity*, which is published by UNESCO as part of its recent World Science Report.

Lenoir's paper provides a timely reminder of the stakes involved in the ethics debate. She reiterates that such debate, far from being an end in itself, provides the means of reconciling human and technical progress, with the ultimate goal of ensuring that such progress contributes to the common well-being, social and democratic progress and the reinforcement of human rights.

Science alone cannot establish a global scheme for society, asserts Lenoir, who argues that ethics provide a 'frame of reference', in particular to help today's society to take responsible decisions about issues that will affect future generations. Such debate is all the more urgent, she says, because scientific advances are no longer automatically considered as a force for progress.

Technology is also being held responsible, she adds, for the degradation of the environment, and increases in health hazards. The Chernobyl disaster for example, marked a turning point in many peoples' perception of the costs and benefits of nuclear power. Scientific progress is also being blamed for dehumanizing society and creating social inequalities both within individual societies, and between the industrialized and developing worlds.

However, the modern ethics movement mainly owes its origins to advances in biology and medicine, in particular the development of techniques of genetic engineering. Bioethics debates are increasingly being translated into legislation in many countries—France, for example, adopted a comprehensive set of bioethics laws in 1994. Today, over 200 national committees have been established to consider the ethical issues raised by biomedical progress.

UNESCO has created the world's first International Bioethics Committee (IBC), a body that is made up of 60 representatives of a diverse range of disciplines and professions from 50 countries. Similarly, the European Union has also set up a group to advise its executive arm, the European Commission, on ethical issues related to biotechnology. Lenoir is chairwoman of both bodies.

The emerging focus of the bioethics movement on protecting human rights and reconciling human and technical progress are perhaps exemplified by the IBC's proposed declaration on the human genome.

This declaration is scheduled to be adopted next year by UNESCO, and may eventually be followed up with a convention that would be binding on its signatories.

The declaration is modelled on the 1948 Universal Declaration of Human Rights, it affirms the principles of the need to respect human dignity to contain technological hazards, and to preserve scientific liberty. The ultimate goal of the declaration, says Lenoir, is to place the human genome firmly in the 'common heritage' of mankind, and to make it subject to international law. As such, the text reaffirms the rights of individuals to preserve their dignity and freedom, condemns discrimination based on genetic characteristics, and rejects genetic reductionizm—the tendency to stigmatize, ostracize or eliminate individuals not meeting a genetic norm.

Lack of cooperation hampers fight against global threats

Governments and scientists need to find new mechanisms to coordinate big-science projects if they are to properly tackle pressing global problems such as the AIDS pandemic, global warming, energy research, and food production. This is one conclusion of a report, *Megascience*, by Thomas Ratchford, an ex-White House official, and Umberto Colombo, a former Italian minister of research.

The report, which is published in UNESCO's new World Science Report, points out that the big science projects needed to address such problems are becoming increasingly expensive at a time when national research budgets are falling almost everywhere. Big science projects include both large coordinated research networks, such as the global research programmes to study climate change or sequence the human genome, and large science facilities such as the European Synchrotron Radiation Facility, Grenoble (France).

Megascience at present is characterized by strong competition among national research groups, increased politicization of funding, and 'erratic decision-making' at the national level. The better alternatives, it says, are improved cooperation, greater international discussion of megascience projects, and perhaps the development of an agreed international budget for such projects. Megascience projects, at least the larger ones, might also benefit by being provided with greater funding stability by establishing them under formal treaty or other agreements among the largest economies, it adds.

Ratchford and Colombo also warn that megascience projects are especially vulnerable under the current conditions of financial austerity. Pressure to reduce public spending, they argue, is increasingly causing

such projects to be judged less on what they might achieve scientifically, and more on what they are likely to cost, and on how they are likely to meet perceived needs of society, such as the provision of new jobs and improved economic competitiveness.

Another threat comes from within the research community itself. Megascience projects are often considered as an unjustified drain on scant resources by researchers working in other areas, who feel that the money could be spent better elsewhere The report, however, dispels this reasoning as a myth arguing that funding for most big-science projects is usually provided as extra money outside of existing research budgets. Indeed, the report points out that when big science projects are cancelled, such as the US Superconducting Super Collider, the money saved is usually reallocated to areas other than research.

In Britain, however, there has been and continues to be a major debate between the funding of international science and national science—both are funded out of the same government subsidy and if, for example, the cost of subscription to an international project rises, then there is less money available for national science.

The report argues that international collaboration in big science projects may be one means for cash-strapped nations to see through the current period of financial austerity. It also provides a means for them to extract better value for money from their individual research efforts. International collaboration also offers other benefits such as the cross-fertilization between scientific communities from a diversity of countries, including smaller nations and those in the developing world.

The report asserts that the time is right for new initiatives in megascience. The authors point out that the political climate is now more conducive to international

cooperation than it has been in the past. The end of the Cold War has abolished much of the rationale for the funding of national cutting-edge megaprojects. Indeed, greater collaboration between geographical blocs has itself become a political goal in the post Cold War world, and science, which is less political than many other issues, is a natural bridge. Moreover, enthusiasm for projects that enhance national prestige is also increasingly succumbing to economic realities.

Conversely, the management of international projects inevitably meets with the realities of global politics, including complex and costly bureaucracies and inefficiencies. The report warns that developing more efficient structures for managing international megascience projects has now become an urgent imperative, given the pressing nature of the global problems that need to be tackled.

Many international organizations are already involved in promoting international collaboration. UNESCO itself, which played a major role in the creation of the European Laboratory for Particle Physics (CERN), today runs several global research and training programmes in ecology, hydrology, geology and oceanography.

In 1992, the Organization for Economic Cooperation and Development (OECO) set up a megascience forum, which acts as a clearing house for information on big science projects, and has recently been given wider powers that may allow it to help provide a more robust and permanent framework for international collaboration.

In Europe, the European Community has also become a major paymaster of collaborative projects. But the report adds that the task of ensuring long-term commitment of resources may be beyond the capacities of existing agencies, while adding that the nature of the global problems being tackled might justify a 'special initiative' on the their part

Sex discrimination impoverishing science

Science and technology remains a man's world. Women remain poorly represented in science and technology jobs, and are more likely to quit the sector than are men. Improving this situation will require countering discrimination against women working in science, and obtaining better representation for women on the high-level bodies that fix research policies. These are the main conclusions of a report by Sandra Harding, Universities of Delaware and UCLA, USA, and Elizabeth McGregor, International Development Research Centre (IDRC), Canada, which is published as part of UNESCO's new World Science Report.

The report asserts that the dice remain loaded against women in educational systems world-wide, particularly in developing countries. Almost two-thirds of the world's illiterate are women. Half those living in developing countries never go to school, while over 100 million children of school age in the world do not have access to the school system; 60 million of these are girls.

Educational opportunities for women continue to be compromised by the decision of parents to only send boys to school or by pressure on girls to marry early according to the report. It adds that women are also often discouraged from studying science and technology, by stereotyped attitudes that say that these 'men's' subjects are unsuitable for women.

Within the scientific establishment, women tend to earn less than similarly qualified men, adds the report. Science is no more understanding of women's need to combine careers and family than other professions, it says, while women scientists suffer isolation in a male-dominated field. Not surprisingly, conclude the authors, women who enter the science and technology system tend to leave more frequently than do men.

Change is unlikely to happen tomorrow, says the report, claiming that governments and research institutions still ignore gender issues. Similarly, the research on gender issues that might help to remedy the situation is only beginning to be recognized as a legitimate activity, according to the report, which adds that tenure review committees nonetheless often discriminate against such research.

Another reason for the continuing neglect of women's issues in science and technology is the quasi-absence of women on the high-level bodies that set policy, argues the report. Similarly, the influence of women is reduced, it claims, because they tend to relegated to less powerful committees, and given smaller research budgets and fewer support staff. The low level of participation of women scientists in regional, national and international policy-making bodies remains an 'invisible problem', says the report, because of the lack of serious attempts to gather information on the extent of the problem.

Greater involvement of women would strengthen science by injecting diversity into what is largely a male-dominated area, argues the report. 'It may not be so much an issue of whether women produce different science, as a principle of producing science relevant to social needs and reflecting all interests of society', it concludes.

***World Science Report 1996**, 356 pp, is published by UNESCO Publishing, Paris; USD 45; ISBN 92 3103220-8*

The Chemical MIME project

Henry S. Rzepa, Peter-Murray Rust† and Benjamin Whitaker‡*

This document is available on-line as http://www.ch.ic.ac.uk/chemime/iupac.html

If you have any comments, please E-mail: any of the principal authors of this document (rzepa@ic.ac.uk, p.murray-rust@mail.cryst.bbk.ac.uk, benw@chemistry.leeds.ac.uk) or send a comment to the discussion forum chemime@ic.ac.uk)

Contents

1. Background and history to the project
2. Why do we need chemical Internet standards?
3. Chemical MIME types included in the May–October 1995 IETF draft
4. New types proposed since the original IETF draft
5. The Chemime discussion list archives
6. Uptake of Chemical MIME usage (Alta Vista statistics)
7. A list of projects utilizing Chemical MIME
8. Software which supports Chemical MIME media types directly
9. Background articles and other information about Chemical MIME

1. Background and history to the project

Prior to 1992, the 'Internet' was essentially a matrix of computer networks bound by a common 'network' protocol and used predominantly as a computer file transfer mechanism and electronic mail carrying mechanism. Standards were in place, but they tended to be generic ones dealing with technical issues. No explicit chemical standards were in place. Around 1993, two new mechanisms were introduced on the Internet.

(a) Electronic mail evolved from purely text based communication, to systems where 'attachments' to the message could be included. For the first time, it became possible to include attachments which could have a chemical content.

(b) A mechanism for document delivery called the World Wide Web was introduced. Here too, a document could be associated with chemical content via a device known as a 'hyperlink'.

It became obvious during 1993 that the enormous potential for exchange of structured information that the Internet now offered would have to be matched by globally accepted standards for such information. At this stage, we considered that 'chemical' information represented a potentially definable class of 'media type' that had certain unique characteristics that would require particular handling by the recipient of such information. We started a project in January 1994 which we called 'Chemical MIME'. This was first announced during the Chemistry workshop at the First WWW International Conference, held at CERN in May 1994.

Our intention was to establish a set of standard 'headers' that would unambiguously identify 'chemical content' in Internet Electronic Mail message bodies and World Wide Web documents. We originally identified a small number of relatively standard file types containing chemical information, which together with the addition of a Chemical MIME header, would enable the content to be sensibly processed by the recipient of the information. Essentially, this was an addition to the MIME standard which had been proposed and ratified via a body called the IETF (Internet Engineering Task Force) in 1993. We initially approached the IETF with our proposal, via a discussion document called an Internet Draft. The first version of this was published during May–October 1994, and a second revised version during April–September 1995. These two proposals each expired after six months of discussion. In July 1995, we presented our case in person at the IETF meeting in Stockholm. Out of this meeting there emerged several conclusions.

- The IETF mechanisms for discussing and accepting such enhancements of the MIME standards were not functioning efficiently at that time.
- The IETF committees were focused largely on Electronic Mail handling and as a result, discussion centred on a relatively nonproductive attempt at semantic distinction between 'chemistry' as a 'subject type' and 'chemical' as a 'media type'. Here, the sociological question of whether all subject disciplines would rush to register their own discipline as a MIME type was the perceived danger
- Application of MIME to the World Wide Web was viewed by some purists as departing from the original strict interpretation of the MIME standard, and the interaction between the two communities appeared strained and at the time unproductive.
- Meanwhile, the original Chemical MIME proposals were widely disseminated throughout the chemical communities, and have been widely adopted via various electronic forums. It is the proposal of the current discussion document to define a set of

*Department of Chemistry, Imperial College, London; †Department of Pharmacology, University of Nottingham; ‡School of Chemistry, University of Leeds, UK.

Chemical MIME standards for endorsement by IUPAC committees.

2. Why do we need chemical Internet standards?

Effective information exchange takes place when everyone uses the same tools. There are a number of ways this can happen, varying from careful planning over several years to the adoption of a *de facto* approach that everyone uses. When organizations try to develop information tools without the general knowledge and consent of the community, great tensions usually result, and it is our intention to try facilitate progress with as little conflict as possible.

Communities are usually suspicious of organizations that 'go it alone' in developing information tools and this often results in competing systems developed under a veils of secrecy; there is a built-in disadvantage to those outside the developer's organization. This is evidenced by the flame-wars that are common on many public newsgroups and discussion groups at present.

Chemistry has inherited a large number of legacy approaches to information and whilst these are useful for some subsets of the discipline, we feel strongly that the tools of the future will only come through public debate and cooperation. Also, however, we need a variety of ideas and approaches so it is valuable to see which ones 'evolve' as well as being planned. If a sub-community finds a useful *de facto* standard, that may well be worthy of recognition as such; but it may also need careful tailoring so that it interfaces well with other areas. This can only come through public activity.

Many tools developed by single organizations in a competitive situation are not future-proof, i.e. they may not be interpretable in a few years' time and the information may be effectively lost. This is particularly likely for binary files, but may also happen when numbers or abbreviations are used. Examples of this are common, and it would be presumptuous to guess which products were still supported in the future.

Terms are often given different semantics or used with default units. It is therefore important to agree with the rest of the community how a term is to be interpreted, and ideally there should be algorithms to convert to related terms.

Guidelines

We propose that those developing information standards commit to the following guidelines:

General

All developers of information tools commit to these guidelines; there should be no reason to depart from them without warning and discussion.

Organizations should be prepared, where appropriate, to enter the standards creation process in a constructive manner.

- Chemical information exchanged in the public arena should follow these guidelines.
- All documentation required to interpret the syntax and semantics of the information in a document should be publicly accessible.
- Documents should be capable of being validated against this documentation.
- Where possible, developers should make code available for reading and writing documents in a given format.
- Where possible, distributors of information should use the chemical/MIME approach described below.
- New technology opens new ways of managing information, some of which may challenge or undermine the guidelines here. All developers should try to anticipate this by raising such issues with the community, and not pre-empt the communal view by inappropriate use of technology.

Chemical/* MIME

A proposal for classifying and regulating the types of chemical document has been submitted to the IETF. A number of existing file types were proposed which have met with wide acceptance in the molecular community. Until the IETF or other body ratifies the proposal, the following guidelines for the use of MIME types are proposed:

- The number of types should be strictly limited. (Usually each type requires specific software to read it, thus placing a burden on readers).
- MIME types should not be used or developed as a means of gaining a market monopoly; it is required that the description of a document's format be made public and reading/writing software is encouraged.
- New versions of existing types must not be introduced without prior discussion and acceptance. This includes clear procedures for naming versions and detailed documentation of revisions.
- New subtypes will be discouraged if there is already a subtype which is capable of carrying that information. chemical/* should not be seen as simply a means of authenticating current legacy systems.
- The use of chemical/* should not be used as a means of adding apparent authority to an organization's project or system if this has not already been discussed. The use of chemical/* in the public arena in ways not sanctioned is deprecated.
- Developers are urged to use mark-up languages where possible (e.g. CIF, ASN.1, CML) and to define the semantics of use (e.g. through glossaries of terms). These definitions should be public, and if possible equivalences to other definitions should be given.

3. Chemical MIME types included in the May–October 1995 draft as part of a 'standards track' process

The following list of Chemical MIME types forms the main body of the IETF Internet draft valid during the period May–October 1995.

Type	Filename extension
chemical/x-cxf	cxf
chemical/x-mif	mif
chemical/x-pdb	pdb
chemical/x-cif	cif
chemical/x-mdl-molfile	mol
chemical/x-mdl-sdf	sdf
chemical/x-mdl-rdf	rdf
chemical/x-mdl-rxn	rxn
chemical/x-embl-dl-nucleotide	emb, embl
chemical/x-genbank	gen
chemical/x-ncbi-asn1	asn
chemical/x-gcg8-sequence	gcg
chemical/x-daylight-smiles	smi
chemical/x-rosdal	ros
chemical/x-macromodel-input	mmd, mmod
chemical/x-mopac-input	mop
chemical/x-gaussian-input	gau
chemical/x-jcamp-dx	jdx
chemical/x-kinemage	kin

5. The Chemime discussion list archives

During the Period November 1994-present, a discussion list has been active for people to discuss various aspects of the proposals. Users can subscribe by sending a message to listserver@ic.ac.uk with the content 'subscribe chemime your name'. The discussions of this forum are archived under http://www.ch.ic.ac.uk/hypermail/chemime/

7. A list of projects utilizing Chemical MIME

1. Original Examples at Imperial and Leeds Universities.
2. NCBI Project at NIH
3. Brookhaven Protein Databank
4. Molecules R Us facility at the NIH
5. Protein Science E-Journal
6. Journal of Molecular Modelling
7. Nature Science Journal
8. Electronic Conferences in Trends in Organic Chemistry: ECTOC-1 and ECHET96
9. Klotho Project at WUSTL.
10. Project CORINA at Erlangen University
11. ChemFinder Project by CambridgeSoft
12. Demos by Daylight Software.
13. Molecule-of-the-Month Collections
14. Chemical and Drug Structure Display at the NIH

8. Software which supports Chemical MIME media types directly

1. *Chemscape Chime by MDLI*: A Netscape plug-in.

9. Background articles and other information about Chemical MIME

1. Antony N. Davies. Internet Chemical MIME. *Spectroscopy Europe* 1996, **8**(1), 42.
2. H. S. Rzepa, B. J. Whitaker, M. J. Winter. *J. Chem. Soc. Chem. Commun.* 1994, 1907.
3. O. Casher, G. Chandramohan, M. Hargreaves, C. Leach, P. Murray-Rust, R. Sayle, H. S. Rzepa, B. J. Whitaker. *J. Chem. Soc. Perkin Trans* 1995, **2**, 7.
4. S. M. Bachrach, P. Murray-Rust, H. S. Rzepa, B. J. Whitaker. *Network Science* 1996, **March**.
5. Maryilyn Dunker, Indiana University. *Chemical Information Viewers: A Collection of programs that can be used with Chemical MIME datasets.*
6. Scott Nelson, Lawrence Livermore National Laboratory. *A Test Page for Checking Your MIME Configurations.*

4. New types proposed since the original IETF draft

Type	File extension	Description and Formal Description	Originator
chemical/x-chemdraw	chm	ChemDraw Format	CambridgeSoft
chemical/x-chem3d	c3d	Chem3D Format	CambridgeSoft
chemical/x-mdl-tgf	tgf	Transportable Graphics Format	MDL Information systems
chemical/x-csml	csml	Chemical Structure Markup Langauage	P. Murray-Rust, R. Sayle, H. S. Rzepa. B. J. Whitaker, *J. Chem. Soc., Perkin Trans* 1995, **2**, 7.
chemical/x-vmd	vmd	VMD—Visual Molecular Dynamics	Andrew Dalke, see http://www.ks.uiuc.edu/Research/vmd/
chemical/x-cml	cml	Chemical Markup Language	Peter Murray-Rust. Developers version 0.7

6. Uptake of Chemical MIME usage (Alta Vista statistics)

The following URL fragments represent Alta Vista (http://www.altavista.digital.com/) searches using the Advanced Query feature after the keyword 'link:' (e.g. link:www.ch.ic.ac.uk). It can report an estimate or actual count of the number of pages pointing to a particular link. This search was performed on 23 July 1996.

URL used for Alta Vista search	Number of other documents with a Hyperlink to this page	Comment on page
'www.ch.ic.ac.uk/chemical_mime.html'	550	One of the two original project pages used to illustrate the use of Chemical MIME-types
'chem.leeds.ac.uk/Project/MIME.html'	400	The second MIME project page
'www.ch.ic.ac.uk/chemime2.html'	250	The original IETF Chemical MIME-types standards document
'www.ncbi.nlm.nih.gov'	8000	NCBI
'www.pdb.bnl.gov'	3000	Brookhaven
'www.prosci.uci.edu'	2000	The Electronic Journal Protein Science
'structbio.nature.com'	900	Nature

Training for the Polish Chemical Industry

Dr Tadeusz Piotrowski

Institute for Industrial Organic Chemistry
Annopol 6, 03-936 Warsaw, Poland

Benefits from Participation in the IUPAC-UNESCO-UNIDO Training Programme on chemical Safety for the Polish Chemical Industry

The concentration of chemical production in small areas, mostly in urban areas containing high concentrations of people, using large amounts of dangerous chemicals and producing serious toxic wastes, causes a great potential hazard to people and to the environment. This is a particular problem in developing countries and in the mid-eastern post-communist countries of Europe. In some regions the situation is alarming.

To prevent such situations giving rise to disasters, IUPAC's Committee on Chemistry and Industry (COCI) has already organized two workshops on safety in chemical production The first such workshop took place in Basle, Switzerland in 1990 and the second in Yokohama, Japan, in 1993.

0n the basis of experience acquired while organizing these workshops, IUPAC, UNESCO and UNIDO established a joint training programme. The aim of this training programme was a systematic transfer of knowledge in the area of process safety and environmental protection from developed countries to developing countries The programme comprises the training of 10–12 trainees each year and will cause a significant increase in the level, and awareness about, chemical safety and environmental protection in these developing countries.

In the first stage of the training programme, 1994, the national adhering organizations of UNIDO selected candidates from China, India, Thailand and Poland. These trainees received training at IUPAC company associates in Germany (Bayer) and Switzerland (Roche and Ciba). The author of this paper, a scientist from the Chemical Safety and Standardization Division of the Institute of Industrial Organic Chemistry, Warsaw, Poland, was placed in Ciba's Unit of Safety and the Environment in Basle, Switzerland. He was a guest of the Explosion Technology/Electrostatics Group headed by Dr Martin Glor. Here the author became acquainted with the latest technology for preventing dust explosions, and the latest innovations in process safety for chemical industries who handle combustible solids in the dusty state. The work in this laboratory involved the examination of the dangerous properties of combustible solids, both on the laboratory and industrial scale, in the big explosion vessels (2.4–25 m^3 volume) at a test site in Zeglingen, near Basle

The important part of this training was the develop-

ment of an acquaintance with a practical use in industry of the results of this research work, mainly in the form of the developed explosion suppression systems tested by the research team. The systems consisted of special explosion detectors, high pressure powder extinguishers and computer-controlled very fast cut-off valves which separate the immediate neighbourhood of the forming explosion from the other parts of the installation. The author examined the explosion properties of dusts in a spherical explosion vessel of 20 L, vapours of combustible liquids in a spherical vessel of 5 L, minimum ignition energy of dusts in MIKE-3 apparatus and took part in the various field tests of the new explosion suppression systems for industry, which needed the use of big explosion vessels of 2.4 m^3, 10 m^3 and 25 m^3.

The other part of the training programme was an introduction to the details of risk analysis as established and used in Ciba. This work put to a good use the tests and examination results made in the laboratories visited by the author. The very substantial was a fact that the programme has not been limited of visiting, looking and discussing. During the time a trainee is with an IUPAC Company Associate, he/she has the opportunity to observe how all aspects of safety and environmental care are managed.

What profit did the author gain from this training programme and his participation in the IUPAC-UNESCO-UNIDO Training Programme on Chemical Safely, and how do these experiences aid the author now in his present post? He saw a modern company with a chemical production plant situated in the heart of a major city, which did not cause problems for the citizens of that city. He became acquainted with the latest research equipment, research techniques and their practical implementation. He has seen the high priority that is attached to safety and environmental protection in industrialized countries. He has also had an opportunity to get to grips with specific technical problems connected with dust explosions and explosion prevention that interested him and to establish contact with key experts in that sphere of science and technology.

However, the most important experience derived from participation in the IUPAC-UNESCO-UNIDO training programme for the Polish chemical industry was the elaboration, on the order of Polish Ministry of Industry and Trade, of the governmental research project on the subject of process safety in chemical industry. This project concerns 'The complete system of identification, evaluation and classification of process hazards in chemical industry compatible with European standards.' The purpose of the project is to work out a method, and define the procedures of the fire and explosion hazard level evaluation for the chemical processes which can cause major hazards for people and the environment. Such an evaluation should take into consideration the dangerous properties of the produced/processed materials, as well as the hazards generated by the specific process conditions. These activities should be closely connected with work on new national laws in that area and on EEC directives adaptation. The project consists of two main tasks divided into stages. 'Methods and procedures of identification, evaluation and classification of the process hazards in chemical industry for preventing technological failures caused by especially dangerous fires and explosions' and 'Standard set of tests and determinations of the fire and explosion indices for material and process hazards'. The complete realization of these projects has been estimated to require about 94 months. The elaboration of the system and its application in the industry should significantly improve the process safety level in Polish chemical plants.

The second important result of the author's training was the preparation a plan for the modernization of the author's own work place. This modernization to consider the importance of minimizing explosion risk. The author has attempted, through the medium of educational seminars and technical talks, to stress the importance to his Polish colleagues of a detailed analysis of explosion risk from whatever cause it may arise in chemical processing.

Recent reports

Terminology for membranes and membrane processes (IUPAC Recommendations 1996)

Synopsis: This project has involved assembling a basic set of terms applicable to non-living membranes and membrane processes. The terms include the key vocabulary used in the literature concerned with scientific, technical and commercial aspects of the membrane field. Processes and membranes based on synthetic or modified natural polymers as well as ceramic and metallic membranes are covered. The resultant terms and their definitions represent a core set that will allow uniform understanding and eliminate most ambiguity or confusion caused by conflicting terminology now in use. The terms and definitions selected for inclusion reflect the majority preference of the membrane community. To avoid irreconcilable differences, definitions

and descriptions involving interpretations of phenomena were minimized. Some terms were deleted in cases where majority preferences were not apparent. This strategy was adopted with the understanding that the current core group of terms, which enjoy majority support, can be augmented as evolution of the field occurs.

This report was prepared for publication by W. J. Koros[1], Y. H. Ma[2] and T. Shimidzu[3] ([1]Department of Chemical Engineering, The University of Texas at Austin, Austin, Texas 78712-1062, USA; [2]Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA 01609-2280, USA;[3]Division of Molecular Engineering, Kyoto University, Yoshida-Honmachi, Sakyo, Kyoto, 606-01, Japan) of the Working party on Membrane Nomenclature from the Commission on Functional Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1996,* ***68****, 1478–1489.*

Critically evaluated propagation rate coefficients in free radical polymerizations—I. Styrene and methyl methacrylate (Technical Report)

Synopsis: Critically evaluated rate coefficients and confidence limits, with derived Arrhenius parameters and confidence ellipses, are reported for the propagation rate coefficients of styrene and methyl methacrylate at low conversion in bulk. Data were obtained by pulsed-laser polymerization in several laboratories, and obey the consistency criteria established for this technique. These results provide useful 'benchmarks' for measurements of propagation rate coefficients by other workers and other techniques.

This report was prepared for publication by Robert G. Gilbert (Chemistry School, Sydney University, NSW 2006, Australia) for the Working Party on Modelling of Kinetics and Processes of Polymerization of the Commission on Polymer Characterization and properties of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1996,* ***68****, 1491–1494.*

Nomenclature for non-linear chromatography (IUPAC Recommendations 1996)

Synopsis: This report summarizes and comments terms and symbols used for the description on non-linear chromatography.

This report has been prepared for publication by Jan Ake Jönsson (Department of Analytical Chemistry, University of Lund, PO Box 124, S-221 00 Lund, Sweden) of the Commission on Separation Methods in Analytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1996, ***68****, 1591–1595.*

Analytical methodology for the determination of aluminium fractions in natural fresh waters (Technical Report)

Synopsis: The distribution among different species, 'speciation', is essential for understanding the toxicity, bioavailability and transport mechanisms for elements in the natural environment. The distribution of aluminium, Al, among different species has been in focus during the last 20 years or so, and many methods for fractionating Al have been developed. Most of them have are operationally defined, since validation of what is really measured in natural systems is very difficult. This review is a thorough and critical survey of the existing methods for Al fractionation in natural waters, that covers the literature up to and including June 1994. The methods have been classified into six groups, according to the principles used: (i) Kinetic or Binding Strength Discriminations; (ii) Ion Chromatographic Separations; (iii) Size Exclusion; (iv) Non-Invasive Methods; (v) Ion Mobility in an Electric Field; (vi) Minimized Disturbance. In addition to this, in order to validate the different techniques, we scrutinize some of the method comparisons published.

This report has been prepared for publication by Nicholas Clarke, Lars-Göran Danielsson and Anders Sparén (Division of Analytical Chemistry, Royal Institute of Technology, S-100 44 Stockholm, Sweden) for the Commission on Microchemical Techniques and Trace Analysis of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1996,* ***68****, 1597–1638.*

Specific problems in the measurement and interpretation of complexation phenomena in seawater (Technical Report)

Synopsis: Characterization of metal complexation phenomena in seawater is a formidable challenge. Adequate characterization of inorganic complexation schemes is currently limited by a paucity of well-defined hydrolysis constant data for chemical species which are important in the weakly alkaline conditions of nor-

mal seawater. Other important problems include the neglect of equilibria involving metals and ligands which form highly insoluble solids, and a poor understanding on the influence of pressure on stability constant behaviour. Characterization of metal complexation by organic ligands in seawater is especially problematic. There is presently a large gulf between laboratory investigations on metal complexation by structurally characterized organic ligands, and investigations of complexation by natural organics whose molecular structure is essentially unknown. In view of the wide variety of techniques used to investigate the complexation behaviour of natural marine organics, and the diverse and occasionally conflicting attributes reported for metal complexation by natural organics in seawater, it would be most valuable if some level of effort were devoted to analysis of shared samples. In view of the multi-faceted strengths of the diverse procedures available for characterization of natural organo–metal interactions, conjugate analysis using a variety of techniques on identical samples seems essential for bringing a reasonable level of constraint to interpretation of complexation observations.

This report has been prepared for publication by Robert H. Byrne (Department of marine Science, University of Southern Florida, St. Petersburg, Florida 33701-5016, USA) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1996,* ***68****, 1639–1656.*

Quantitative analysis of a $PbO–SiO_2$ glass by electron microprobe (Technical Report)

Synopsis: A standard glass sample denoted by the National Institute of Standards and Technology as K-456 was analysed by an international collaborative team. The results of quantitative determinations of the two oxide glass components, PbO and SiO_2, are compared and the deviations from the standard values are calculated. Methods of preparation, conditions of quantitative determination and procedures used for the evaluation of the results are also summarized

This report has been prepared for publication by J. Matousek[1], V. Hulinsky[1], R. Metselaar[2] and J. Cornish[3] ([1]Institute of Chemical Technology, Prague, Czech Republic; [2]Technische Universiteit Eindhoven, Eindhoven, Netherlands) for the Commission on High Temperature and Solid State Chemistry;[3] Trinity College, University of Dublin, Dublin, Ireland) of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1996,* ***68,*** *1657–1663.*

A collaborative study of the structure and rheological properties of EVOH/SMA (ethyl–vinyl alcohol copolymer/styrene–maleic anhydride copolymer) blends produced by reactive extrusion (Technical Report)

Synopsis: Blends of ethylene–vinyl alcohol copolymer (EVOH) and styrene–maleic anhydride copolymer (SMA) have been produced by reactive extrusion and characterized in terms of their rheology, phase morphology and the degree of covalent bonding interaction (ester linkages) between phases, as determined by FTIR.

Strongly synergistic behaviour in terms of viscosity and melt elasticity was seen in all blends, for low frequency dynamic and low shear rate capillary tests, the largest increase occurring in blends containing 50–60% EVOH. Finely dispersed droplet phase morphologies were seen in most of the blends, the minor phase forming the dispersed phase. However, the blends containing 50–60% EVOH were co-continuous or partly co-continuous; it was also notable that the blends containing 60% EVOH exhibited a surprisingly low value of Melt Index. Evidence of covalent bonding was apparent in all blends, the highest interaction levels again being seen for the 50–60% EVOH blends, despite a very low anhydride/alcohol molar ratio (only 0.5). Increased mixer speed and vacuum venting during processing also improved reaction levels.

These findings suggest that the availability of reactive groups is restricted by the phase morphology of the blend during production. As a result, more reaction occurs at or near co-continuous phase compositions, where the surface area is maximized. The synergistic behaviour in viscosity and elasticity can be seen as consistent with the observed increased bonding levels, which cause more efficient stress transfer into the dispersed phase.

This report has been prepared for publication by P.S. Hope[1], J.G. Bonner[1] and J.E. Curry[2] ([1]BP Chemicals Ltd, Applied Technology, PO Box 21, Bo'ness Road, Grangemouth, FK3 9XH, UK; [2] Werner & Pfleiderer Corporation, 663 East Crescent Avenue, Ramsey, NJ 07463, USA) for the Working Party on Structure and Properties of Commercial Polymers of the Commission on Polymer Characterization and Properties of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1996,* ***68,*** *1665–1682.*

News

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* (1995) **17**(6), 215–226. The IUPAC Secretariat have been notified of the following changes:

Dr Athel Cornish-Bowden has ceased to be Chairman of JCBN.

Dr J.M. Fremy (Secretary, Commission VI.5), Tel: +33 (1) 55 76 21 60; Fax: +33 (1) 55 76 27 06.

Prof. J.E. Guillet, (Secretary, Division IV), Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6.

Prof. Ian M. Mills (Chairman, IDCNS), Fax: +44 (0) 118 9316331.

Dr Jaroslav Stejskal (Secretary, Commission IV.2), Tel: +420 (2) 360 341; Fax: +420 (2) 367 981.

Maison de la Chimie Foundation Prize

The Board of the *Foundation de la Maison de la Chimie*, Paris, France, has decided to award in 1998 the *Grand prix de la Foundation*. This prize, created in 1985, is worth FF 150 000, which makes it one of the most significant prizes awarded in chemistry and the application of chemistry. Previous recipients of this prize have been: Prof. Paul Hagenmuller, 1986; Dr Michael Elliot, 1989; Prof. Rudolf Wiechert, 1991; Prof. Mark Vol'pin, 1994, and Prof. Claude Hélène and Prof. Peter B. Dervan, 1996.

The prize is awarded to reward original work in chemistry of benefit to mankind, society or nature. The prize for 1998 will be FF 150 000 and will be awarded to one or several persons irrespective of nationality. Entry forms may be obtained from:

Foundation de la Maison de la Chimie, 28 rue Saint-Dominique, 75341 Paris, Cedex 7, France. Tel.: +33(1) 4062 2700; Fax: +33(1) 4555 9862.

All entries must be presented through a learned society or through a national or international scientific organization. Completed entry forms and a report on the work of the candidate must be registered by the secretariat of the *Maison de la Chime* before 1 May 1997.

Entries will be judged by an international jury composed of a Chairman and eight members recognized for their work in different fields of chemistry. The 1998 jury includes the two previous laureates.

The award ceremony will take place on 20 January 1998, at *Maison de la Chimie*, Paris, when the successful laureate will give a presentation of the award-winning work.

IXth International IUPAC Symposium on Mycotoxins and Phycotoxins, Rome, Italy, 27–31 May 1996

The IXth International IUPAC Symposium on Mycotoxins and Phycotoxins was held in Rome, Italy from 27 to 31 May 1996 as the latest in a series of very successful symposia organized by the Commission on Food Chemistry of the Division of Chemistry and the Environment of IUPAC.

Mycotoxins and phycotoxins are important catego-

39th IUPAC General Assembly, 23–30 August 1997, Geneva, Switzerland

Payment for Titular Members

Previously, the reimbursement of expenses incurred by Titular Members participating in IUPAC General Assemblies was handled in two parts. Travel claims were dealt with by the Oxford Secretariat before the General Assembly and subsistence was reimbursed during the General Assembly.

For the Geneva General Assembly, however, both travel and subsistence will be paid from Oxford, to those who have requested payment in advance, well before the start of the General Assembly (Spring, 1997). Thus, it is recommended that Titular Members return their Claim Forms promptly to the Secretariat in Oxford. On this claim form you should ignore the phrase in parenthesis in the subsistence section—claims will in fact be paid by cheque from Oxford, not in cash in Geneva. However, those Titular Members who request payment of travel in Swiss Francs (CHF) in Geneva will receive their subsistence payment in Geneva—cheques drawn on the Banque Cantonale de Genève, will be distributed by the IUPAC Secretariat.

Fig. 1 Chairpersons of the Organizing Committees of IUPAC Symposia on Mycotoxins and Phycotoxins. From left to right: Dr Pieter Steyn (South Africa, 1985), Dr Marina Miraglia and Dr Carlo Brera (Italy, 1996), Dr Magda Carvajal (Mexico, 1992), Dr Yoshio Ueno (Japan 1988).

ries of natural toxins occurring world-wide in foods, feeds, water and seafood. The awareness that these contaminants play an aetiological role in human and animal diseases has led international organizations such as IUPAC to stimulate scientific co-operation and research in this field.

Between 1972 and 1992 IUPAC, through its Commission on Food Chemistry, organized eight symposia on mycotoxins and phycotoxins. During the first 10 years the symposia focused mainly on mycotoxins and were held in Sweden (1973), Poland (1974), France (1976) and Switzerland (1978). From 1985 onward, phycotoxins were given more prominence and the symposia shifted from Europe to South Africa (1985), Japan (1988) and Mexico (1992).

The latest symposium was co-sponsored by IUPAC, the Standards, Measurements and Testing Programme of the European Commission and the Food and Agricultural Organization of the United Nations and was held in the Istituto Superiore di Sanita of the Italian Ministry of Health, which is the main institute of technical-scientific research in Italy giving advice on public health. Both the Chairperson and Secretary of the Organizing Committee, Dr Marina Miraglia and Dr Carlo Brera, were from this Institute and they were ably assisted on the Organizing Committee by Dr J. Gilbert from the UK, Dr H. van Egmond from the Netherlands and by C. Calicchia, R. Onori and L. Toti from Italy and Dr C. Canet representing the FAO.

The IXth International IUPAC Symposium on Mycotoxins and Phycotoxins was held over 5 days and included:

1. A Sampling Workshop
2. A FAO/IUPAC Workshop dealing with practical considerations on food analysis for mycotoxins in developing countries.
3. A session on the Standards, Measurements and Testing Programme (SM & T) of the European Commission.
4. A Forum for Italian Scientists on the importance of mycotoxins for human and animal health.

The scientific tone of the Symposium was set by the Keynote Speaker, Dr J.D. Miller of Agriculture Canada, who stressed the importance of mycotoxin and phycotoxin exposure for both human and animal health especially in developing countries. He drew attention to the economic consequences of mycotoxin contamination both in terms of human Disability Adjusted Life Years lost in developing countries due to diseases modulated by mycotoxins as well as the direct agricultural losses due to animal deaths and reduced animal productivity. He concluded that ' the single most important thing that could be done for the human diet and grain-based agriculture would be the elimination of mycotoxins'.

The different sessions of the symposium focused attention on various aspects of the chemistry of mycotoxins and phycotoxins such as:

1. The natural occurrence in foods and feeds in different countries.
2. Methods to monitor the presence in foods, feeds and biological fluids.
3. Toxicokinetic studies.
4. Toxic mechanisms of action at the molecular level.
5. Management strategies for the prevention and control of contamination.
6. Toxicity and carcinogenicity studies.
7. Human risk assessment studies.

Fig. 2 Delegates attending the IXth International IUPAC Symposium on Mycotoxins and Phycotoxins in Rome, Italy during May 1996.

Scientific contributions on mycotoxins included presentations on aflatoxins, fumonisins, ochratoxin and trichothecenes while those on phycotoxins focused on the marine toxins such as Okadaic acid, Diarrhetic Shellfish Poisoning (DSP) toxins and Paralytic Shellfish Poisoning (PSP) toxins while several con-

tributions were made on the freshwater toxins produced by cyanobacteria, the microcystins.

One of the major features of the symposium in Rome, which was attended by more than 300 delegates, was that scientists from many countries participated in the proceedings. Over the years this symposium series proved to be truly international in character and this was again reflected in the programme of the symposium in Rome. Out of a total of 271 scientific contributions 47 were lectures on mycotoxins, 24 were lectures on phycotoxins while there were 179 and 21 posters on mycotoxins and phycotoxins, respectively. The outstanding features, however, were that the authors included scientists from 48 countries and that 137 contributions out of a total of 271 were from countries outside Western Europe or North America. The symposium therefore succeeded in bringing scientists together and creating a forum for the transfer of information to developing societies.

The proceedings of this symposium will be published by Alaken Publishers and should be available during 1997.

Reactivity of solids: past, present and future

The concept of reactivity seems to have been formulated in chemistry near the beginning of the 20th century. At that time, when speaking of the reactivity of a substance one meant the ability of individual molecules to take part in various chemical reactions, as well as the rate of these reactions. Indeed, the chemical properties of gases and liquids are, to a large extent, determined by the characteristics of the individual molecules. However, when the same atoms and molecules form solids, the cooperative interactions may make the properties of a solid noticeably different from those of the individual molecules. Hence, the reactivity of solids is essentially not the same as the reactivity of molecules.

Our understanding of reactivity has undergone an evolution over time. Not a very long time ago, reactions of solids such as decomposition or interaction with gases were well known. However, it did not seem to be obvious that reactions between solids could be at all possible. A statement, 'Corpora non agunt nisi fluida' is ascribed to Aristotle. It was not until the beginning of this century that it became evident that solid state reactions do take place. This has stimulated the first special studies of solid state reactions, and the first attempts to understand the mechanisms of these processes, and the factors determining the reactivity of solids. It is important to remember that at the time of these initial studies of solid state reactions, most of the presently used tools of studying solids were not available, for example, the X-ray diffraction techniques were not developed and the crystal structures of solids were not known! Understanding of the physics of the solid state at the beginning of this century was also very different from what it is now.

More and more experimental data were accumulated, which showed clearly that chemical reactions of solids are different in many respects as compared with reactions of liquids and gases. Reactivity of a solid has proved to depend on the 'biography' of the solid, i.e. on the method of preparation, storage conditions, preliminary treatment, etc. It turned out that kinetics of a solid state reaction cannot be described adequately only by indicating the degree of transformation as a function of time. Solid state reactions tend to be heterogeneous, the reaction rate usually depends on the site in a solid sample and therefore not only time, but also spatial coordinates are required for an adequate kinetic description.

Studies of chemical reactivity of solids were greatly influenced by the achievements in the developing of the physical theories of solids. As understanding of solid state physics progressed, the theories of chemical reactivity of solids were also revised.

The first theories of solid state reactivity were based on considering the idealized crystal lattice. Then it turned out that real solids are never perfect, and every solid contains deviations from its idealized structure, termed defects. These defects can play an important role in solid state reactivity. First, defects can serve as potential centres at which the reaction starts. This phenomenon is usually termed as the localization of the process. Secondly, defects are important for the transport processes in solids, such as diffusion of ions and electron transfer through a layer of product. Many of the first detailed studies of the reactivity of solids were aimed at elucidating the role of defects in solid state reactions, and even to suggest some semi-quantitative theories. Even today, many of the ideas proposed in the 1930s–1950s have not lost their value. As examples, one can mention: A. Hedvall's model interpreting the changes in the reactivity of a solid at the point of phase transition; the idea of C. Wagner to treat the thermodynamics of point defects in solids in terms of the theory of

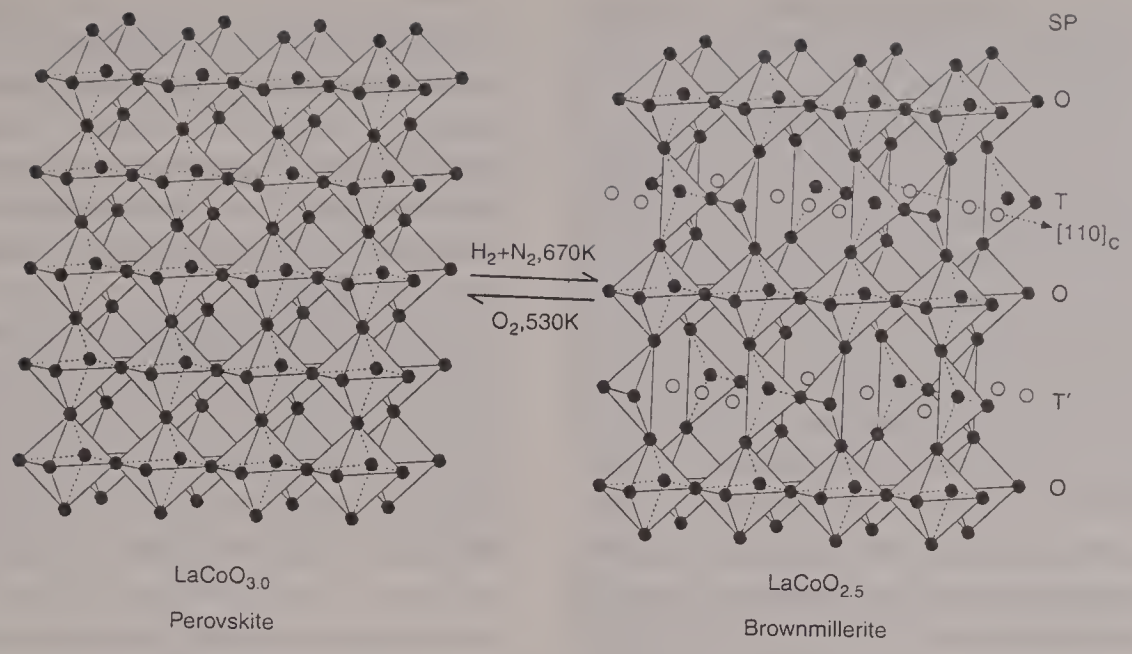


Fig. 1 Reduction of $LaCoO_3$ to $LaCo_2O_5$ (From K. Vidyasagar, A. Reller, J. Gopalakrishnan and C.N.R. Rao, *J. Chem. Soc. Chem. Commun.*, 7–8 (1985)).

the electrolyte solutions; the model of N. Mott and P. Gurney describing the processes in photographic systems; Bernard's model of oxidation of metals and of the reduction of metal oxides; the shear structures proposed by J. Anderson, etc. These highly original studies can now be considered as classical. They impress by their clarity, coherence and the breadth of generalization. The authors of these studies did not have the experimental tools that we have now.

By the late 1940s, it became clear that not only the chemical composition and the idealized crystal structure of a solid are essential for its reactivity, but also the types and concentration of the defects. At first, defects, especially the non-equilibrium ones, were expected to increase the reactivity in all cases, since each defect is a distortion of crystal structure and accumulation of the defects results in an increase in the energy of the solid. However, the interrelationship between the reactivity of a solid and the concentration of the defects in it turned out to be not that simple. More and more experiments showed that some defects did not affect the reactivity at all, whilst others could even inhibit the reaction. The effect of the defects on a particular solid state reaction is interrelated with the participation (direct or indirect) of these defects in this reaction. The experimental study of the effect of various types of defects on a solid state reaction proved therefore to be helpful in elucidating the reaction mechanism and finding the methods of the control of the reactivity. The theories used to describe thermodynamics and kinetics of solid state reactions were also to be modified in such a way, so as to take into account the role of the defects. As just one of the numerous examples one can cite the concept of an 'active state' of a solid (referring to a solid with a non-equilibrium concentration of defects), used when considering the thermodynamics of solid state processes.

One of the most characteristic features of solid state reactions (as compared with reactions in gases or in liquids) is that they are usually heterogeneous. Since the reactivity at different sites in a solid is often different, the reaction rarely starts simultaneously throughout the bulk or over the entire surface of a solid. Although this fact was mentioned as early as, for example, Faraday's working diaries, it seems to be Langmuir who first paid proper attention to the fact that a solid state reaction tends to be the reaction at the interface between the starting reactant and the product. The interface is often also referred to as the reaction zone. Understanding that heterogeneous solid state reactions are reactions at the interface was essential for the development of the kinetic theories of these processes. The 'topokinetics' aimed to take into account the variation of the size of the 'reaction zone' with time when calculating the reaction rate constants. The theory has borrowed some concepts from the theory of crystal growth and provided a set of the equations, which are now considered to be 'classical' (and, unfortunately, as often happens with 'classical equations', are often applied without a proper justification). Topokinetics flourished at the middle of this century, but at the present time the interest in it has considerably decreased. This may be, at least partly, because some of the basic postulates of topokinetics turned out to be inconsistent with the experimental data. A real solid state reaction turned out to be even more complicated than a process of crystal growth. Also, the forms of the feedback in the interface processes can be more diverse.

The first studies of solid state reactions paid most at-

tention to the striking differences between homogeneous reactions in gases or liquids on one side, and heterogeneous reactions in solids on the other side. This seems to be quite natural. Nevertheless, this trend can no longer form the basis for the progress in solid state chemistry. Critical analysis should be followed by a positive synthesis, and the time to throw stones must give way to the time to collect them. A theory of the reactivity of solids is still to be worked out. This theory will be of value not only for solid state chemists but also for specialists in physical, inorganic and organic chemistry. Chemistry is only artificially subdivided into separate 'subdisciplines'. It seems to be high time to start searching for links between the commonly accepted concepts of 'classical molecular chemistry' and the ideas of solid state chemistry.

Another important point in developing the theory of reactivity of solids is related to possible industrial applications. Solid state reactions are already used in technologies, and it is important to be able to control their course. The demand of new technologies that would be ecologically 'cleaner' and also advantageous economically is permanently growing. In many cases this means the necessity to develop 'dry technologies', based primarily on solid state reactions without using liquids at all. It is a commonplace that progress in fundamental science is usually related to the demands of industry, but this obviously is true for solid state science also. I am sure that although up to now attempts of technological applications of solid state reactions were only sporadic, an increasing interest in these reactions from industry will also stimulate the developments of the fundamental aspects of solid sate science.

It is also a commonplace that each science is progressing owing to the joint efforts of many scientists. Therefore, it is important that scientists have an opportunity to exchange ideas, to review the results and to outline the prospects for the future. As far as reactivity of solids is concerned, this opportunity is provided by organizing international symposia, which have been held regularly every 4 years since 1948 (Paris 1948, Gothenburg 1952, Madrid 1956, Amsterdam 1960, Munich 1964, Schenectady 1968, Bristol 1972, Gothenburg 1976, Cracow 1980, Dijon 1984, Princeton 1988, Madrid 1992, Hamburg 1996).

Another way to review previous studies is to publish books, monographs and collective monographs. I would like to mention the 'classical' books of the 1950s, which were the 'milestones' in the development of the theory of reactivity of solids, i.e. the books by J.A. Hedvall, K. Hauffe, W.E. Garner and P. Budnikov. In the 1960s– 1980s some more books appeared (for example, those by P. Barret, V. Boldyrev, M. Bulens, B. Delmon, K. Meyer, D. Young, H. Schmalzried, M. Brown, D. Dolimore and A. Galwey). Special issues of journals were also devoted to the problems related to reactivity of solids, for example a special issue of the *Journal de Chimie Physique* edited by P. Barret and B. Delmon (1986). The present book—issued in the IUPAC series *Chemistry in the 21st Century*—pursues the same goal. This is a collection of articles written by experts from different countries. The authors have tried to provide a wide overview on the progress in the fields, in which they are recognized to be leaders, to evaluate the present state of research and the prospects for the future. The book covers the problems related to the hierarchy of the defects in the solids, the kinetics of chemical reactions in solids and the reactions in solid matrices. It also considers in more detail some particular types of heterogeneous reactions, for example thermal decomposition and dissolution of solids, interaction of solids with gases, as well as solid-solid reactions. Further on, homogeneous solid state reactions and chemical reactions in organic solids are considered. Special chapters are devoted to the problems related to the application of solid state reactions in inorganic synthesis and in the manufacture of new materials.

Of course, it is impossible within the scope of one book to cover the wide range of problems related to the reactivity of solids. Thus, for example, the book does not have contributions related to the applications of the theory of the reactivity of solids in experimental geology and mineralogy, despite an obvious progress achieved in this field. Regrettably, because of the sudden death of Professor M. Figlarz, the problems related to 'soft chemistry' are also not covered in the book. Also, a chapter devoted to the applications of the theory of reactivity of solids in catalysis and in the industry of pharmaceuticals has not been included, although interesting results have been obtained recently in these fields. Being the editor/compiler of the book, I am well aware of all these shortcomings. At the same time, I hope the reader will understand that the editor of this kind of book has limitations, and cannot do everything absolutely to his liking. As the ancient Romans said: 'Feci quod potui, faciant meliora potentes'.

V.V. Boldyrev

The following is a list of the chapters, together with the authors' names, which appear in this volume:

Hierarchy of defects in crystals and reactivities of solids. V. Gutmann and G. Resch

The reactivity of solids in thermal decomposition (crystolysis) reactions. A. K. Galwey

Problems of reactivity in the dissolution of inorganic solids. M.A. Blesa

Some data on surface properties and reactivity of metal oxides. L.C. Dufour

Processes at interfaces during solid state reactions. M. Martin

Modern tendencies in heterogeneous kinetics of solid

state decomposition reactions. N. Lyakhov
Homogeneous solid state reactions. E.V. Boldyreva
Kinetics of the simplest radical reactions in solids. V. A. Tolkatchev
Reactivity of organic solids: past, present and future. G.R. Desiraju and B.S. Goud
Chemical strategies for the synthesis of metal oxides. C.N.R. Rao
Low-temperature materials syntheses. R. Roy
Reactivity of solids and new technologies. V.V. Boldyrev

Reactivity of Solids: Past, Present and Future, A Chemistry for the 21st Century Monograph, edited by V.V. Boldyrev, Blackwell Science, 1996, xii + 291 pages, ISBN 0-86542-687-2, price USD 79.50 (hardback).

Science international: a history of the International Council of Scientific Unions

Our subject is really the betterment of the human condition, but our material is individual scientists choosing to work together and trying to take science beyond the limitations of individual effort. The number of scientists in the world, acting in many ways, increased greatly in the 20th century. Of them an influential few (relatively few but amounting to some thousands) took part in the events set out here which have involved members of a distinctive type of international organization.

Two words occur repeatedly in these pages: Academy and Union. Each has been used many times to label a voluntary gathering of men and women of like interests. The Academies discussed here do not always bear that word in their titles, but all represent the scientific communities of individual nations, men and women of several callings working together to give the people of the national communities to which each owes his or her way of life a single scientific voice. Groups of scientists all over the world, of a single disciplinary commitment, have devised ways of working together regardless of their personal national affiliation, the international communities they have developed using the title of Union. Such Unions can exist independently, but what we are concerned with here is the way the Unions, through the International Council of Scientific Unions (ICSU), have developed a way of working with each other and with the national academies. Most of the increasing number of personal participants have been occupants of academic posts, in universities and research institutes, but they have been men and women whose interests lay well beyond the individual pursuit of abstract knowledge. The base of their involvement has been that they have cared for the effective sharing of new knowledge, within a particular discipline and, more important, between disciplines. The peak of their involvement is their concern, not always expressed or felt, for the common future of humankind, which has meant that they have created lines of communication, not only with each other, but also with the world of politics and economics. This book has to begin long before the present form of ICSU and must deal with its predecessor bodies, the International Association of Academies and the International Research Council. Indeed, as the story begins some of the nations and their scientific academies did not exist. We can therefore only go as far as the present position and hold back from speculation. So much is seen to have changed that it would be unwise to predict what might happen next.

Dr Frank Greenaway

Science International: A History of the International Council of Scientific Unions, by Frank Greenaway, Cambridge University Press, 1996; xi + 279 pages; ISBN: 0521-58015-3 (hard cover).

Fig. 2 ICSU headquarters.

Use of the World Wide Web for access to IUPAC documents

Use of the Internet, and particularly the World Wide Web, has been expanding at an enormous rate—see the report on the UNESCO/ICSU sponsored conference on electronic publishing earlier in this issue. While it is clear that IUPAC must make use of this new, and widely effective, mode of communication, it is less clear exactly how best to use it. The Committee on Printed and Electronic Publications (CPEP) was asked both to establish the Home Page and to suggest guidelines for the use of those committees and individuals in IUPAC who have information (both 'official' and unofficial) to disseminate.

In drawing up these guidelines, CPEP has tended to stress open and free (no-cost) distribution over pay-per-view or access limited to those who have paid for the print equivalent. In so doing, CPEP recognizes that it may, over time, be necessary to protect the revenue of IUPAC's printed publications through more restricted access to some of the Web pages. Nevertheless, at this early stage of our experience with electronic distribution, we have thought it preferable to encourage very broad usage, so that both the Union and chemists world-wide have incentive to learn how to use this exciting new medium to advantage.

1.0 Material published in *Chemistry International*

In principle, any material published or due to be published in *Chemistry International* may be displayed at the IUPAC Web site (at present maintained by the Royal Society of Chemistry at Pipex, Cambridge, UK; URL: http://chemistry.rsc.org/rsc/iupac.htm), at the discretion of the IUPAC Information Officer.

2.0 Recommendations published in *Pure Appl. Chem.*

In principle, all recommendations and technical reports published in *Pure Appl. Chem.* will be made freely available via World Wide Web, by one of the following methods.

2.1 The file should preferably be mounted at the IUPAC Web site either as part of the directly available HTML-formatted Web material or in a separate directory accessible to FTP. To facilitate these arrangements, the document author should provide the computer-readable version, with a description of the file type (e.g. HTML or Microsoft Word RTF) at the same time as final camera-ready copy is submitted to Pure Appl. Chem.

2.2 Alternatively, the file can be mounted by the author or an associate at his/her local site as a fully HTML-formatted Web document. An example is the Glossary of Class Names mounted at Queen Mary and Westfield College, London. In this case the IUPAC Web Home Page will contain a hypertext link to the appropriate URL address (e.g. http://www.qmw.ac.uk/~ugca000/iupac.html). Full reference should be made to the original publication and the IUPAC copyright statement should be included. Documents made available initially in this way should be transferred eventually to the IUPAC Web site, in order to ensure their long-term availability.

2.3 The file can be held in native word-processor or compound document format (compressed if appropriate) at the local site, and made available for transfer by ftp. The IUPAC Web Home Page will contain a hypertext ftp link to the file.

3.0 Recommendations on nomenclature and symbolism published in compendium form (the IUPAC Colour Books)

This is material from which IUPAC expects to derive income from hard- copy sales. Recommendations not previously published in Pure Appl. Chem. can be made available as outlined in sections 2.1–2.3, but not until twelve months after publication of the book.

4.0 Provisional recommendations

Past experience with IUPAC drafts has shown that provisional recommendations are often used by the community regardless of their status. The possibility of making such drafts more widely available by the use of the Internet should therefore be viewed with caution. However, the advantages of reaching a wider community for review of drafts are considerable. The following arrangements will therefore be made.

4.1 The IUPAC Web site will display titles and synopses of provisional recommendations (as published in *Chemistry International*) as HTML files. Those requiring a copy of the draft (on Paper) will be instructed to send a request to the appropriate regional document distribution centre at the address given: where possible

this will be facilitated by an E-mail: hypertext link. All distribution drafts should carry the prominently displayed message: Provisional Recommendations—FOR COMMENT ONLY, NOT TO BE CITED, on each page.

4.2 In addition, at the discretion of the Chairman of the Commission concerned, the document may be mounted as a native or HTML file at the author's local site as outlined in section 2.2, with a hypertext link from the displayed title and synopsis on the IUPAC Home Page. If a document is made readily available for downloading in this way, its provisional status should be made clear by the prominently displayed message: Provisional Recommendations—FOR COMMENT ONLY, NOT TO BE CITED. This message should appear as a 'watermark' (preferred) or as text inserted at frequent intervals.

5.0 Recommendations published jointly with other international organizations

IUPAC will make available joint publications in the ways outlined in sections 2.0 and 3.0 provided that all the material concerned is IUPAC-approved. Hypertext links from the IUPAC Home Page will be given for material at sites maintained by other organizations. In cases where joint publications contain material not approved by IUPAC or outside its control, this fact will be made clear in the specification of the hypertext link.

6.0 Pre-provisional draft recommendations

Some Commissions and Working Parties will wish to use the World Wide Web as a medium for circulation of and comment on draft material at an earlier stage, before submission to IDCNS. This is potentially a valuable means of facilitating input to IUPAC proposals, and will be allowed at the discretion of the Commission Chairman. However, such an arrangement should be managed via facilities available to Commission members, without involving the IUPAC Web site. Documents mounted on the Web in this way should be clearly marked with a draft number and date, and each page should carry the prominently displayed text: DRAFT FOR COMMENT: NOT TO BE CITED. Password-protection facilities should be used if available, to ensure that access is restricted to members of the group concerned. Text in such drafts should avoid phraseology susceptible to extraction and quotation out of context as IUPAC recommendations (e.g. IUPAC-approved values are...).

Recommendations prepared by Dr Alan McNaught, Secretary, IDCNS

Conferences

New Approaches in Polymer Synthesis and Macromolecular Formation, St Petersburg, Russia, 16–20 June 1997

IUPAC
SPONSORED

The Institute of Macromolecular Compounds of the Russian Academy of Sciences and the Chemistry Department of Saint-Petersburg State University are continuing the series of St Petersburg meetings on macromolecules. The International Symposium 'New Approaches in Polymer Synthesis and Macromolecular Formation' will be held in St Petersburg, Russia, from 16 to 20 of June, 1997. Saint Petersburg is one of the most beautiful cities in the world. The House of Scientists of St Petersburg (the former Grand Duke's palace) is chosen as a venue of the Symposium.

The main aim of the Symposium is to discuss the modern problems of polymer synthesis and macromolecular formation. These areas of polymer chemistry have been changed dramatically during the last two decades. New molecular architecture, supramolecular chemistry, achievements in traditional polymer synthesis, catalysis in polymer preparation, synthesis of polymers with use of oligomeric synthons, synthesis of hybrid polymers and other problems of modern synthetic polymer chemistry are planned to be discussed at the Symposium:

- New approaches in chain- and stop- growth polymerization Catalysis in polymer synthesis
- New macromolecular architecture
- Non-traditional methods of macromolecular formation

The Symposium program will include about 20 invited lectures of 30 min, oral communications and poster presentations.

English is the working language of the Symposium.

No translation service will be provided.

The registration fee is USD 300 for regular participants and USD 100 for students. For the IUPAC affiliate members a 10% reduction of the registration fee is settled. The registration fee for accompanying persons is USD 50. As recommended by IUPAC, to facilitate the participation at IUPAC-sponsored symposia the registration fee for scientists from East European countries is reduced to the student-level registration fee. Various social events are planned for accompanying persons: sight-seeing tours of the city and its suburbs, excursion to the world-renown museum 'The Hermitage', theatre performances.

The participants will be offered hotels of varying costs and a student hostel.

The city is situated on the same latitude as Helsinki and Oslo. It has a humid maritime climate. It is famed for its White Nights. They begin on the 20th–21st of May, when the sun sinks no lower than 9°. The White Nights are not really nights at all, but a slight dusk, lasting a mere 30–40 min, which lends the city's streets, squares and embankments an unforgettable beauty.

For further information, please contact: *Irina Rovalenko, Symposium Coordinator, Institute of Macromolecular Compounds, Bolshoy pr. 31, St Petersburg, 199004 Russia. Tel.: (812) 213 1070; Fax: (812) 218 6869. E-mail: IMC@MACRO.SPB.SU*

3rd International Congress on Recovery, Recycling and Re-integration (R'97), Geneva, Switzerland, 4–7 February, 1997

IUPAC
SPONSORED

R'97 Congress—the world's most comprehensive event in Integrated Resources Management (IRM)—will:

- strike a balance between science, industry and legislation
- consider ecological, economic and social factors and implications
- lead to environmentally and economically acceptable solutions, through the active involvement of all interested parties
- show latest developments in recovery, recycling and re-integration technologies.

A wide base of co-organizers and supporting bodies ensure a high quality platform at R'97 for debating, exhibiting and communicating processing technology, their ecological, economic and social implications. The papers to be presented have been selected by an international Scientific Panel of experts, and are of the highest quality. The selection criteria embraced scientific content, feasibility and effective realization. In contrast to other conferences, emphasis is not on materials and products, but on topical subjects (such as logistics and thermal processes) of relevance to all materials and products. A full morning of workshops will provide an opportunity to concentrate the discussions on specific products and materials, such as building or fibres materials. The schedules ensure that one can progress from the general to the specific, and that there is minimal overlap of two topics for interested groups such as, for example, concepts and ecological consequences or logistic networks and separation technologies.

What sets R'97 apart from other events?

The difference rests in the high level of scientific content, the international character, the multidisciplinary participation, the efficient tools of communication and, last but not least, a wide majority of satisfied attendees in R'95. The event will be combined with an international exhibition.

1. The Scientific Excellence and Practical Relevance
Chaired by Prof. H. Ursprung, Swiss Secretary of State for Science and Education, R'97 is a non-profit event, where 49 distinguished scientists from 16 countries ensure the scientific quality and practical relevance of the papers and posters.

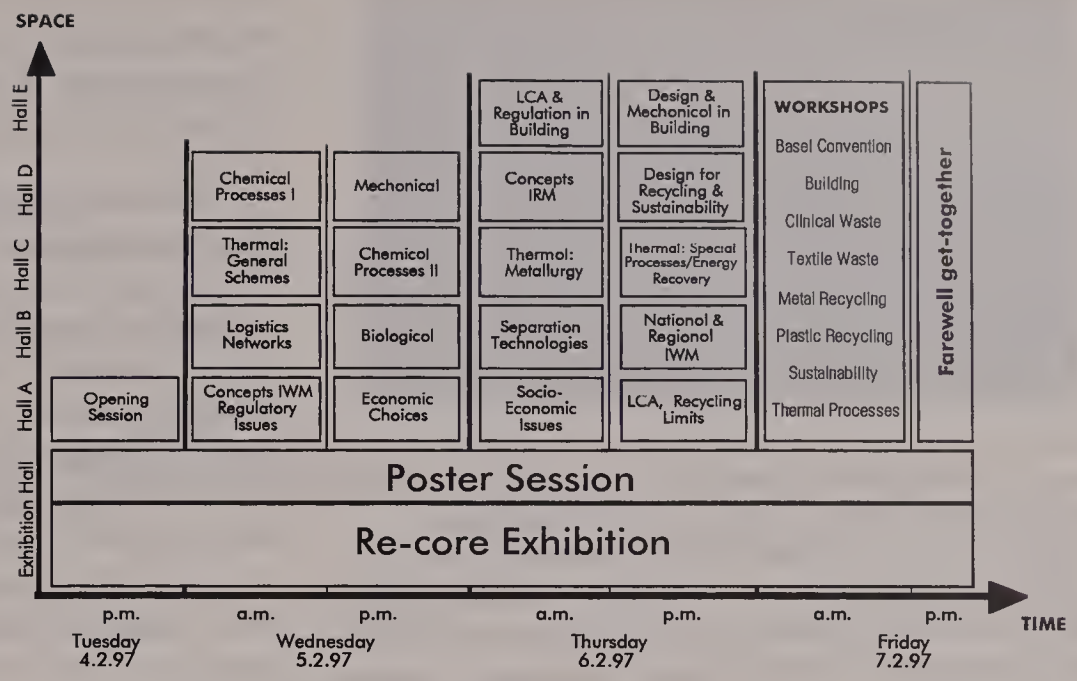
2. R'97 Congress—a World Event
More than 350 papers from 45 countries in all continents have been submitted. Delegates from more than 60 countries are expected to attend R'97. More than 30 international organizations are supporting actively R'97. A Steering Committee which includes more than 40 industry organizations have helped to shape the programme, by indicating and contributing to the most topical issues in the field of Integrated Resource Management (IRM). International organizations (UNEP, SBC, etc.) will diffuse congress findings in all member countries.

3. Multidisciplinarity
Multidisciplinarity begins with the choice of co-organizers from science, industry (ICC) and international and national legislation (UNEP, SBC, UBA)—the three pillars of the congress. Multidisciplinarity is assured by the topics covered: all recovery, recycling and re-integration processes—mechanical, chemical, biological and thermal, logistical; economic, legal and social issues are addressed. All waste streams and natural resources will be covered in R'97.

4. Communication
Communication tools of R'97, i.e. oral and poster sessions with proceedings, workshops and the exhibition guarantee an intense and fruitful dialogue on IRM issues.

Relevant papers on IRM issues will be distributed by

Programme structure



the Scientific Panel according to their suitability either to oral or poster sessions. Workshops allow short presentations and comprehensive dialogue on the most topical issues in IRM as follows: Basel Convention, Sustainability, Metal Recycling, Plastic Recycling, Fibre Recycling, Thermal processes, Building, Clinical Waste.

More than 800 delegates, 150 international journalists attended R'95. 95 per cent of these judged R'95 as very good. We expect more at R'97! Press releases will be mailed to 1200 international titles, 7 press conferences shall be organized in UK, Paris, USA, Berlin, Zurich, Budapest, Geneva and Stockholm. 300 journalists shall be invited to R'97. More than 15 million potential readers, listeners and watchers were reached 1995.

5. Exhibition: Re-core

Re-core stands for the core of communication on recovery, recycling and re-integration. The heart of the exhibition is the communication market place. Its mission is to ensure the most comprehensive dialogue between all sectors and display exhibits, as well as posters elaborating on processes, concepts, product designs, etc., e.g. solutions for the problems posed by IRM and environmental added values. Layout, modular stand concepts and involved costs, ultimately the convenience of R'97 shall be the unique selling proposition (USP) of Re-core. A completely equipped stand (3×3 m) costs CHF 2970.

Re-core will support sales efforts of the industry and will promote their philosophy to solve global and local IRM related problems. A high scientific and technological content will distinguish Re-core from other, conventional trade fairs.

33rd International Conference on Co-ordination Chemistry—*The chemistry of metal ions in everyday life* (XXXIII ICCC), Florence, Italy, August 30–September 4, 1998

IUPAC SPONSORED

The 33rd in the series of International Conferences on Co-ordination Chemistry will take place in the *Centro Internazionale Congressi Firenze* in Florence, Italy, in 1998. For further information, please contact:

33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy.

36th IUPAC Congress—*Frontiers in chemistry, new perspectives for the 2000s*, Geneva, Switzerland, 17–22 August, 1997

IUPAC SPONSORED

IUPAC NSCS

Registration fees for the 36th IUPAC Congress are as follows:

Registration and payment	Before 15 May 1997	From 16 May 1997
Regular participant	CHF 550	CHF 650
Young scientist*	CHF 200	CHF 300
IUPAC affiliate	CHF 495	CHF 585
Accompanying person	CHF 50	CHF 50
Day tickets		
Regular participants	CHF 350	
Young scientists	CHF 100	

* Non-industrial participants under 30 years of age (born

before 1 January 1967) qualify for the young scientists fee, but proof date of birth, for example, a photocopy of a passport, should be enclosed with the registration form.

For further information and further updates please read the following WWW site: http://www.unige.ch/sciences/chimie/IUPAC/IUPAC.html Otherwise, please contact: Prof. Jacques Weber, Section de Chimie, University of Geneva, 30 Quai Ernest Ansermet, CH-1211 Geneva 4, Switzerland.

Third World Congress on Emulsions, Bordeaux, France, 23–26 September, 1997

IUPAC
SPONSORED

Emulsions play a major role in road maintenance works, as well as in the manufacture of odourless paints, lipstick, beauty cream, perfume and nail polish, not to mention film, mayonnaise and other sauces. Over the last few years, the scientific domains linked to emulsions have been marked by rapid fundamental development, which will certainly yield numerous industrial applications.

This congress will provide a platform for scientists from both academic and industrial backgrounds to promote their work in emulsions and the application of emulsion technology. Four themes are defined:

- Formation and preparation of emulsions
- Characterization, Long-term stability—Rheology
- Emulsion behaviour
- Industrial applications—case histories—new developments and new constraints

Plenary lectures will be given by renowned scientists in the field of emulsions. The lectures invited to participate in the workshops will be selected from amongst those authors who submit papers.

For further information, please contact: *CME, 50 place Marcel-Pagnol, 92100 Boulogne-Billancourt, France. Tel: +33 (1) 47 61 76 89; Fax: +33 (1) 47 61 74 65.*

Environmentally Sustainable Manufacture as a Competitive Advantage, San Francisco, USA, 13–17 April 1997

IUPAC
SPONSORED

An American Chemical Society (ACS)/IUPAC/Chemical Manufacturers' Association (CMA) Symposium, 14–15 April 1997, San Francisco, CA, USA.

With the rapid development of new and ever changing technologies, industrial products and practices inevitable generate materials potentially hazardous to public health and to the environment. Regulation is designed to balance the progress of the industry with the life-sustaining needs of the environment. This concept of sustainable manufacture has become one of the most important challenges for the chemical process industry and has offered the potential for some of the greatest rewards in our increasingly competitive market. The chemical process industry, has however, often perceived environmental and health regulations as barriers to productive research and development. The purpose of this symposium is to discuss relevant issues and to recommend methods by which regulation may serve as a source of competition. Regulation will be analysed in terms of an incentive/disincentive capacity world-wide. The symposium will recommend areas for research and development and product development, make suggestions for the development of environmentally sustainable processes, and propose methods for competing in the domestic and global marketplace.

Environmentally Sustainable Manufacture as a Competitive Advantage: Symposium Technical Programs:

Session A: Demand for Products in the Chemical Industry

Session B: Risk based Decision Making (Cosponsored by CMA)

What risk issues need to be considered when innovating new products? How can risk be reconciled with public perception?

Session C: Business Needs in Environmentally Sustainable Manufacture

Develop a structure for integration of new environmental concepts into business. Examples are:

- Full cost accounting
- Life cycle-analysis
- Green labelling
- Green competition
- Marketing opportunities
- Effect of world competition
- ISO 14000 Environmental Management Standards
- Small companies vs. big companies

Session D: Governmental Incentives and Disincentives

Define positive governmental role with respect to:

- Tax incentives

- Antitrust
- Regulators' successes
- Regulatory failures
- Opportunities for government
- World regulatory equalization
- Regulatory effects on world competition

Session E: Human Health and Environmental Health Issues

Analyse issues arising from and suggest solutions to:

- New unit processes
- New engineering practices
- New Chemistries
- Intentional Standardization
- Case histories

Session F: Implementation in Industry

Further information may be obtained from: *Dr A.M. Ford, Gulf Coast Hazardous Substance Research Centre, Lamar University, PO Box 10613, Beaumont, 77710-0613, Texas, USA. Tel: +1 409 880 8768; Fax: +1 409 880 2397.*

Conference calendar

1997

Thermodynamics

5–8 January

International Symposium on Chemical and Biological Thermodynamics. Amritsar, India.

Prof. Bhajan Singh, Department of Chemistry, Guru Nanak Dev University, Amritsar-143005, India. Tel: +91 (183) 258845. Fax: +91 (183) 258820. E-mail: bhajan@gndu.ernet.in

Recycling

4–7 February

International Recycling Congress (R'97). Geneva, Switzerland.

Dr A. Barrage, c/o LPM Limited, Tannenweg 10, CH-5712 Beinwil, Switzerland. Tel: +41 (62) 7715555. Fax +41 (62) 7715564. E-mail: ipmbar@dial.eunet.ch

Further information about R'97 may be found on their Home Page: http://www.r97.ch/r97

Safety in chemical production

13–17 April

3rd IUPAC Workshop on Safety in Chemical Production: Environmentally sustainable Manufacture of Competitive Products. San Francisco, USA.

Dr A. M. Ford, Gulf Coast Hazardous Substance Research Centre, Lamar University, PO Box 10613, Beaumont, Texas 77710-0613, USA. Tel: +1 409 880 8768; Fax: +1 409 880 2397.

High temperature materials chemistry

19–23 May

9th International Conference on High Temperature Materials Chemistry (HTMC IX). Pennsylvania State University, PA, USA.

Prof. Karl E. Spear, Materials Science & Engineering Department, Pennsylvania State University, 118 Steidle Building, University Park, PA 16802, USA.

Bioorganic chemistry

1–6 June

4th International Symposium on Bioorganic Chemistry. Biarritz, France.

Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45–4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Molecular architecture for degradable polymers

10–14 June

International Symposium on Molecular Architecture for Degradable Polymers: Molecular Design of Polymeric Materials of Tomorrow. Stockholm, Sweden.

Prof. Ann-Christine Albertsson, Department of Polymer Technology, KTH, Royal Institute of Technology, S-100 44 Stockholm, Sweden. Tel: +46 (8) 7908274. Fax: +46 (8) 100775.

Polymer synthesis

16–20 June

International Symposium on New Approaches in Polymer Synthesis and Macromolecular Formation. St. Petersburg, Russia.

Mrs. Irina Kovalenko (Symposium Coordinator), Institute of Macromolecular Compounds, Bolshoy pr. 31, 199004 St. Petersburg, Russia. Tel: +7 (812) 2131070. Fax: +7 (812) 2186869. E-mail: imc@macro.spb.su

Ionic polymerization

7–11 July

International Symposium on Ionic Polymerization. Paris, France.

Prof. F. Cheradame, CNRS, BP 28, 2 rue Henri Dunant, 94320 Thiais, France.

Recycling of polymers

14–17 July

38th Microsymposium on Macromolecules, Recycling of Polymers.

Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Organometallic chemistry

20–25 July
9th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis. Göttingen, Germany.
Dr J. Belzner, Institut für Organizche Chemie der Georg-August-Universität Göttingen, Tammanstrasse 2, D-37077 Göttingen, Germany.

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules, Surface and Interfacial Phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, The University of Tokyo, Hongo, Tokyo, Japan.

Plasma chemistry

18–22 August
13th International Symposium on Plasma Chemistry. Beijing, China.
Dr Lin He, The Chinese Society of Theoretical & Applied Mechanics, 15 Zhong Guan Cun Road, Beijing 100080, China.

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
36th IUPAC '97, c/o AKM Congress Service, PO Box 37, CH-1218 Le Grand-Saconnex/GE, Switzerland. Tel: +41 (22) 7611661. Fax: +41 (22) 7611662.

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion.

Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile.
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel: +56 (2) 6811644. Fax: +56 (2) 6812108. E-mail: jcostama@lauca.usach.cl

Polymers

25–28 August
12th Bratislava Conference on Polymers 'Modified Polyolefins for Advanced Polymeric Materials'. Bratislava, Slovak Republic.
Prof. E. Borsig, Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 842 36 Bratislava, Slovak Republic.

Spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997 (CSI). Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel: +61 (3) 98193700. Fax: +61 (3) 98195978.

Emulsions

23–26 September
2nd World Congress on Emulsion: Industrial Applications of Emulsions. Bordeaux, France.
Mr A. Le Coroller, Directeur-Général, CME, 50 place Marcel Pagnol, 92100 Boulogne-Billancourt, France. Tel: +33 (1) 47617689. Fax: +33 (1) 47617465.

Biodiversity and Bioresources

23–27 November
International Conference on Biodiversity and Bioresources—Preservation and Utilization. Phuket, Thailand.
Prof. Yongyuth Yuthavong, National Science & Technology Development Agency, Gypsum Metropolitan Tower, 18th Floor, 539/2 Sri-Ayudhya Road, Rajdhavee, Bangkok 10400, Thailand.

1998

Trace element speciation

4–7 May
1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences. Munich, Germany.
Dr P. Schramel, GSF-Forschungszentrum für Umwelt und Gesundheit, GmbH, Institut für Ökologische Chemie, Neuherberg, D-85758 Oberschleissheim, Germany.

Organic synthesis

30 June–4 July
12th International Conference on Organic Synthesis. Venice, Italy.

Prof. C. Scolastico, Dip.to di Chimica Organica e Industriale, Università di Milano, Via G. Venezian 21, I-20133 Milano, Italy.

Macromolecules

20–23 July
18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.
Dr Jaromir Lukás, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague 6 Petriny, Czech Republic.

Chemical thermodynamics

26 July–1 August
15th International Conference on Chemical Thermodynamics. Porto, Portugal.
Prof. M.A.V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal.

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr John F. Gibson, Secretary (Scientific), The Royal Society of Chemistry, Burlington House, London W1V OBN. Tel: +44 (171) 4378656. Fax +44 (171) 7341227.

Physical organic chemistry

16–21 August
14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.
Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento di Química, 88040-900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy. Tel: +39 (55) 2757549. Fax: +39 (55) 2757555.

Natural products

October
21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.
Prof. Xiao-Tian Liang, Institute of Materia Medica, Chinese Academy of Medical Sciences, 1 Xian Nong Tan Street, Beijing 100050, China.

2000

Macromolecules

9–14 July
MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.
Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90–363 Lodz, Poland. Tel: +48 (42) 819815. Fax: +48 (42) 847126.

Biotechnology

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHAEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.

International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

President: A. E. FISCHLI (*Switzerland*)
Vice-President: J. JORTNER (*Israel*)

Secretary-General: E. D. BECKER (*USA*)
Treasurer: J. M. WARD (*UK*)

IUPAC Secretariat

Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK.
Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.
Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Neue Schweizerisches Chemische Gesellschaft **(Switzerland)**
Türkiye Kimya Dernegi **(Turkey)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1997, Vol. 19, No. 1 (January)

1 A major event for Swiss chemistry
Jacques Weber

6 Secretary General's Column
Edwin D. Becker

7 Photochemistry in Italy

12 News from the International Organization for Chemical Sciences in Development (IOCD)

14 World Science Report 1996

17 The Chemical MIME project
Henry S. Rzepa, Peter-Murray Rust & Benjamin Whitaker

20 Training for the Polish Chemical Industry
Tadeusz Piotrowski

21 Recent reports

24 News

26 Reactivity of solids: past, present and future

30 Use of the World Wide Web for access to IUPAC documents

31 Conferences

35 Conference calendar

Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Blackwell Science

0193-6484(199701)19:1;1-G

Printed in Great Britain by Alden, Oxford, Didcot & Northampton

ISSN 0193-6484

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

1997, Vol. 19, No. 2 (March)

Blackwell Science

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

ACTING EDITOR: Mike Ward
SECRETARIAL ASSISTANT: Mary Patterson
PRODUCTION EDITOR: Howard Waller

All correspondence to be addressed to The Editor, Chemistry International, IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK. Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk and http://chemistry.rsc.org/rsc/iupac.htm

Editorial Advisory Board

Chairman:	E. D. BECKER	*Secretary-General*	G. SOMSEN	*Division I*
	E. BUNCEL	*CHEMRAWN Committee*	G. J. LEIGH	*Division II*
	A. SMITH	*Committee on Chemistry and Industry*	G. SAVELLI	*Division III*
	D. H. M. BOWEN	*Committee on Printed and Electronic Publications*	A. ABE	*Division IV*
			F. INGMAN	*Division V*
	I. M. MILLS	*Interdivisional Committee on Nomenclature and Symbols*	T. R. ROBERTS	*Division VI*
			(To be appointed)	*Chemistry and Human Health*
	M. E. PESTANA	*Committee on Teaching of Chemistry*		

Subscriptions

Six issues of *Chemistry International* will be published bimonthly in 1996. The 1996 subscription rate including postage is GBP 68.50 (UK and overseas except North America) or USD 106.00 (US and Canada). The individual subscription rate is GBP 27.50 (UK and overseas except North America) or USD 39.50 (US and Canada). Microfiche subscriptions are available simultaneously with the printed edition, and microfilm at the end of the subscription year. Subscription orders may be placed directly with IUPAC's official publisher, Blackwell Science Ltd, PO Box 88, Oxford, UK; E-mail: journals.cs@blacksci.co.uk. Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Advertising. Enquiries should be sent to The Editor, Chemistry International, at the above address, or the Advertising Manager, Blackwell Science Ltd, Osney Mead, Oxford OX2 0EL, UK. Telephone: +44 (0) 1865 206206, Telex 83355 Medbok G, Fax +44 (0)1865 721205.

Despatch. The news magazine is despatched within Europe by surface mail, to other continents by various forms of air-speeded delivery: to the US* by air freight for forwarding by periodicals post, to India by air freight for guaranteeed local delivery, and to all other countries by Accelerated Surface Post.

Reproduction of Articles

Unless there is a footnote to the contrary, reproduction or translation of articles in this issue is encouraged, provided that it is accompanied by a reference to the original in *Chemistry International*. The Blackwell Science logo is a trade mark of Blackwell Science Ltd registered at the United Kingdom Trade Marks Registry.
This journal is included in the ADONIS service, whereby copies of individual articles can be printed out from compact discs (CD-ROM) on demand.

*Periodicals postage paid at Rahway, NJ. Post Master, send address changes to *Chemistry International*, c/o Mercury Airfreight International Inc., 2323 Randolph Avenue, Avenel, NJ 07001, USA.

Front cover: Prof. V.A. Koptyug and Lord (Prof. Alexander) Todd. Recently deceased. See page 51.

International Union of Pure and Applied Chemistry

Introducing the Working Party on Spectroscopic Data Standards (JCAMP-DX)

Antony N. Davies and Robert Lancashire†*

Introduction

The correct transport of scientific data between diverse computer systems and software packages is an essential element of the work of a modern integrated laboratory. This has been addressed by two reports from different working groups within the Physical Chemistry Division, Commission on Molecular Structure and Spectroscopy in recent years [1,2].

Both of the reports recommended adoption of a data transfer standard known as JCAMP-DX after the Joint Committee on Atomic and Molecular Physical Data, Data Exchange. Following several meetings with the IUPAC Databases Committee it was decided that, in order to avoid competing development work on the same standard, an agreement should be drawn up between the JCAMP executive and IUPAC. This agreement committed the IUPAC Committee on Printed and Electronic Publications (CPEP) to set up a Working Party to support and develop the JCAMP-DX range of standards in return for financial support from the JCAMP organisation.

Who's who on the Working Party

The working party has been very lucky in recruiting many of the people who have been developing the use of JCAMP-DX data standards world-wide.

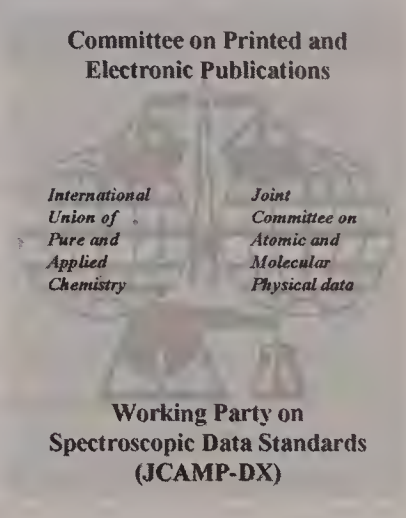
In the USA Bob McDonald, an author of the first JCAMP-DX standard for infrared spectroscopy [3] had been pushing the adoption of these standards and publishing test data sets. He has also developed the use of the Internet for information on the JCAMP-DX standards with a very extensive reference site at:

http://members.aol.com/rmcdjcamp/index.htm

*ISAS, Inst. für Spektrochemie und Angewandte Spektroskopie, Bunsen-Kirchhoff-Str. 11, 44139 Dortmund, Germany.

†Department of Chemistry, University of the West Indies, Mona, Kingston 7, Jamaica.

Readers should note that the figures which accompany this article have been downloaded from the World Wide Web, and may not be of the highest quality.


Committee on Printed and Electronic Publications
International Union of Pure and Applied Chemistry
Joint Committee on Atomic and Molecular Physical data
Working Party on Spectroscopic Data Standards (JCAMP-DX)

Within the European Community the standard had been adopted for food research within the Quest 'Quality Established through Spectroscopic Techniques' project. Leading roles in this project were played by Peter McIntyre of the University of Glamorgan, UK and Doug Rutledge of the Institut National Agronomique in Paris, France. An extended and unified version of the standard for food research was written and an extensive software suite developed to support this use.

The largest spectroscopic database project in recent years, the German government 'Informationssystem Spektroskopie' adopted the JCAMP-DX standards. It was used for data exchange between various project partners as well as for downloading data from the online version of the 'SpecInfo' databases available over STN International.

During this project the next two Standards were published, JCAMP-DX for Nuclear Magnetic Resonance spectroscopy in 1993 [4] and JCAMP-DX for Mass Spectrometry in 1994 [5]. Both protocols were co-authored by Tony Davies, ISAS, Inst. für Spektrochemie, Dortmund, Germany, who is chairman of the IUPAC Working Party and Peter Lampen who now works for the Deutsche Forschunganstalt für Lüft- und Raumfahrt in Berlin, Germany.

Further activities within this project saw software written to automatically correct faults in commercial implementations of the standards. Reports were also generated for spectrometer manufacturers detailing any errors found in their implementations of the protocols.

The explosive development of the Internet for scientific data exchange has revealed a deficit in tools for handling scientific data that are Internet active. The work of Henry Rzepa of Imperial College, London, UK and his colleagues on the Chemical MIME has provided the groundwork allowing other groups to make up this deficit. JCAMP-DX is one of the Chemical MIME types defined by within Chemical MIME. Henry is not a member of this working party but is also leading a parallel

The JCAMP-DX Working Party hard at work on Day 1. From left to right: Chris Muir (UWI), Peter Lampen, Tony Davies, Peter McIntyre, Robert Lancashire, Doug Rutledge, Bob McDonald.

working party on Chemical MIME reporting to the CPEP.

Robert Lancashire of the University of the West Indies (UWI), Mona, Jamaica started using the JCAMP-DX standards as the only reliable method of moving spectroscopic data from his spectrometer and into other applications such as spreadsheets. This interest developed into writing Windows programs to handle and display spectra via the JCAMP-DX standards. His group is now very active producing plug-ins and helper applications as well as Java scripts for JCAMP-DX standards to run with commercial Internet browser packages. This allows scientists to place spectroscopic data in the IUPAC recommended format on the Internet and it can be handled as spectra and not as purely graphical data.

First Meeting at UWI, Mona, Jamaica

Robert Lancashire hosted the inaugural meeting of the Working Party on the 9–15 December 1996. Although most of the work of the Working Party will be carried out electronically it was thought that it would be profitable for the first meeting to be face to face. Despite the excellent weather a large number of topics were covered during the week which will lead to a number of publications.

Generic JCAMP-DX Version 5.0

One of the more important publications to be prepared by this working party is the definition of a generic data exchange standard. This standard known as JCAMP-DX version 5.0 has been around in draft format for several years and was the basis of the two more recent standards for NMR and MS. That this standard has not yet reached publication has caused difficulties for those trying to implement the two newest standards. The Working Party managed to advance the document so that publication in *Pure and Applied Chemistry* can be expected later this year.

A standard file format for nuclear magnetic resonance spectroscopy: JCAMP-DX V.5.01

Following publication of the JCAMP-DX for NMR file format specification in 1993 requests for additions to the protocol were made for applications not originally covered. After careful consideration, it has since become apparent that a few minor modifications will significantly increase the range of possible applications. The Working Party assessed these modifications and they have been detailed in a paper for publication in *Pure and Applied Chemistry*.

The major points covered included pulse sequences, extensions to the allowed axes labelling, more detailed chemical shift referencing, magic angle spinning and sample description labels. This publication will also give an example of the official NTUPLE JCAMP-DX definition as applied to NMR-FID data.

Exchange, interpretation and database-search of ion mobility spectra supported by the JCAMP-DX data format

Despite the rather long-winded title this is a new JCAMP-DX standard protocol for Ion-Mobility-Spectrometry (IMS). The Working Party also has the role of supporting developments of new standards and with this in mind this new draft standard was scrutinised. It is important to bear in mind when assessing such drafts that the use of the generic keywords does not contradict any usage in standards already published. New data type specific information, in this case information that is only relevant in Ion-Mobility Spectrometry, must also be handled in accordance with the Generic JCAMP-DX guidelines.

A range of changes that needed to be incorporated into the protocol before it could be resubmitted for acceptance as a new JCAMP-DX standard have been

The JCAMP-DX Working Party at rest on Day 7. Back—left to right: Peter McIntyre, Doug Rutledge, Bob McDonald, Peter Lampen. Front—Tony Davies.

made. It is hoped that this new protocol should also reach publication in 1997.

A Report on the implementation of the JCAMP-DX format: Comparison between two commercial software packages

Following up on previous work supporting manufacturers in their implementation of the JCAMP-DX standards two implementations by a single manufacturer were studied as well as the interaction between the two software packages. A report was completed detailing areas where the Working Party thought changes should be adopted and this will shortly be submitted to the manufacturer for comment.

One interesting error which appeared during this study was the use of the Microsoft Windows International settings which allows for replacement of periods by commas as separators in real numbers. This appears to be a problem local to Windows software but it is not global to all the software we have looked at running under this operating system. The problem appears when Windows runs with European language versions where, for example, 0.5 in English would be written as 0,5. This is of course unacceptable for an international electronic scientific data exchange standard as files written using the comma as separators would be unreadable by any other system not using this option. Strangely in the data file exported in this manner not all the real numbers in the file were in this format!

Future work

The Working Party will be busy for the early part of 1997 getting the documents mentioned above ready for publication. Following the publication of the Generic Standard an advanced protocol based on the JCAMP-DX version 5.0 will be developed for multi-dimensional molecular spectroscopy data sets. This is being pushed hard because of the lack of a standard to store large, multi-dimensional spectroscopic data sets (image cubes) required for remote sensing interplanetary exploration missions. The Working Party is working to a very tight budget and one of the developments which will also be investigated will be the use of the Internet for video conferencing or for voice-only conferences to save on travel money.

References

1 JCAMP-DX: A standard form for exchange of infrared spectra in computer readable form (Recommendations 1991). *Pure Appl. Chem.* 1991, **63**, 1781–1792.

2 C. Wilkins. Guidelines on solution nuclear magnetic resonance in computerized databases, *Pure Appl. Chem.* 1995, **67**, 593–596.

3 R.S. McDonald & P.A. Wilks. JCAMP-DX: A standard form for exchange of infrared spectra in computer readable form. *Appl. Spectrosc.* 1988, **42,** 151–162.

4 A.N. Davies & P. Lampen. JCAMP-DX for NMR, *Appl. Spectrosc.* 1993, **47**, 1093–1099.

5 P. Lampen, H. Hillig, A.N. Davies & M. Linscheid. JCAMP-DX for mass spectrometry. *Appl. Spectrosc.* 1994, **48**, 1545–1552.

PAC Review

***Pure and Applied Chemistry* (PAC) is the official journal of IUPAC. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in PAC are published in *Chem. Intl.* in the section Recent Reports. In this section we take a brief look at the symposia and lectures published in recent issues of PAC.**

The October 1996. **68**(10), issue of *Pure and Applied Chemistry* contains the texts of the plenary and invited lectures presented at the Sixth International Congress on Automation and New Technology in Clinical Laboratory held in Sitges, Barcelona, 2–4 November, 1995. The Congress was organized by the IUPAC Clinical Chemistry Division, in conjunctions with the International Federation of Clinical Chemistry, the Forum of European Societies of Clinical Chemistry, and Sociedad Espanola de Bioquimica Clinica Y Patalogia Molecular.

Aims, objectives and work program of ISO/TC212 D. M. Jeffers (York Hospital, 1001 S. George Street, PO Box 15198, York, PA 17405-7198, USA)

Standardization has been an important activity for

many centuries. The development of laboratory medicine has depended upon the availability of standardized materials for the preparation of reagents, the publication of standard methods and procedures, the acceptance of standard characteristics to define bacteria and tissue cells, the acceptance of standard nomenclature to report laboratory findings and numerous other criteria and systems to help assure the usefulness of laboratory data.

In his paper, Jeffers noted that the inaugural meeting of the International Organization for Standardization (ISO) Technical Committee 212 (ISO/TC 212) on Clinical laboratory testing and *in vitro* diagnostic systems took place in Philadelphia, PA, USA, on 31 May though 2 June 1995. The secretariat of ISO/TC 212 has been assigned by ISO to the American National standards Institute. Committee membership includes 20 participating member countries and 12 observer members. Jeffers further reported that the committee recommended a structure composed of three working groups: Quality Management in the Clinical Laboratory; Reference Systems; and *In vitro* Diagnostic Products.

In order to take advantage of the vast amount of work that has already been done and published in the focused areas, and avoid unnecessary duplication, a number of liaison relationships were recommended. Category A liaison is utilized for organizations which can make an effective contribution to, an participate actively in, the work of the technical committee. Such liaison includes exchange of documents and invitations to meetings. Jeffers noted that the following organizations have been selected for category A status:

WHO—the World Health Organization
EDMA—the European Diagnostic Manufacturers Association
ICSH—International Council for Standardization in Haematology
IFCC—International Federation of Clinical Chemistry
IUPAC—International Union of Pure and Applied Chemistry
WASP—World Association of Societies of Pathology
ECLM—European Confederation of Laboratory Medicine
ICTH—International Committee on Thrombosis and Haemostasis

Internal liaison has been requested between ISO/TC 212 and ISO/TC 48 (Laboratory glassware and related apparatus); ISO/TC 76 (Transfusion, infusion and injection equipment for medical use); ISO/TC 176 (Quality management and quality assurance); and ISO/REMCO (ISO Council on Reference Materials). Jeffers also noted that representatives from the European Committee for Standardization (CEN) were present at ISO/TC 212's inaugural meeting. CEN/TC 140 (*In vitro* diagnostic systems) is engaged in a number of projects that could either be included in the ISO/TC 212 work programme or submitted to parallel approval under CEN 'ead, according to the provisions of subclause 5.2 of the Vienna Agreement on technical cooperation between ISO and CEN.

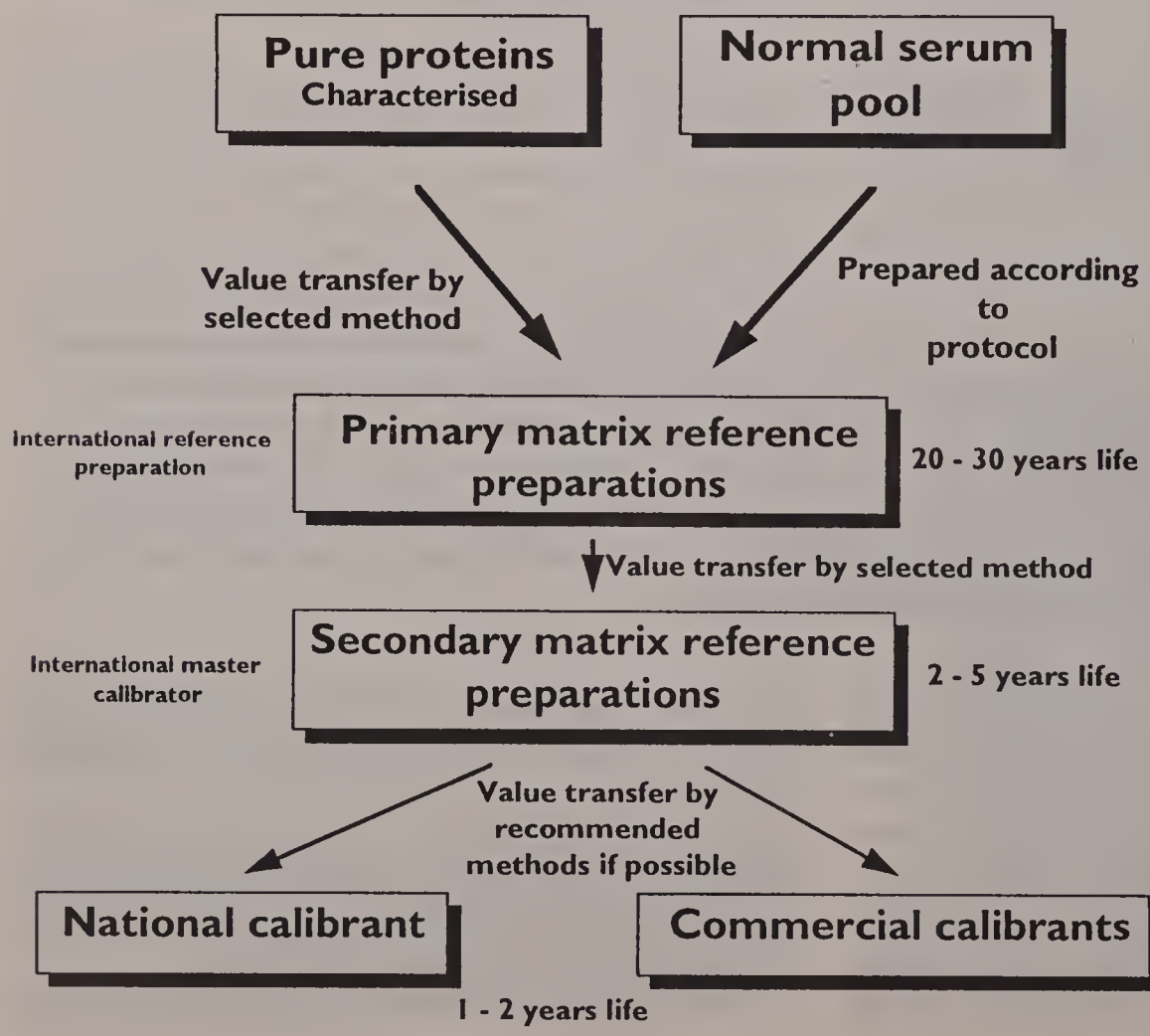


Fig. 1 Classification of international. national and commercial plasma protein reference materials.

Recommended working groups of ISO/ TC 212

Working group 1—Quality Management in the Clinical Laboratory pre- and post-analytical procedures for the clinical laboratory Clinical laboratory safety Quality assurance, including external quality assessment and internal quality control, and accreditation for clinical laboratory medicine Ethics in laboratory medicine

Working group 2—Reference Systems Contents and description of reference measurement procedures and reference procedures utilizing nominal and ordinal scales Contents and description of reference materials Requirements for laboratories performing reference procedures

Working group 3—*In vitro* Diagnostic Products. Identification and determination of analytical and clinical performance goals for laboratory methodologies Determination of desirable performance criteria for blood glucose monitor systems for use in diabetes management Recommendations for validation of user quality control Symbols used in labelling of *in vitro* diagnostic products

The impact of regulations, accreditation standards, and healthcare reform on laboratory practice in the United States P. Bachner (University of Kentucky Medical Center, 800 Rose Street, Dept of Pathology, Room HA609, Lexington, KY 40536-0084, USA).

Professional standards of laboratory practice in the USA are partially derived from regulatory and accreditation standards of the federal government as well as those of non-government organizations and professional societies. According to Bachner, the most important standards that determine daily practice in USA laboratories are those of the federal government (Clinical Laboratory Amendments of 1988, or CLIA88), the Joint Commission on Accreditation of Healthcare Organizations (JCAHO) and the College of American Pathologists (CAP). Hospital and laboratory inspection and accreditation programs of the latter two organization are recognized separately by the Federal Government though an arrangement known as 'deemed status'.

Bachner reported that the implementation of the CLIA88 regulations has had a profound impact on laboratory practice in the USA and has forced the voluntary private sector organizations such as the CAP and the JCAHO to revise their standards and modify their practice to achieve equivalency. Continuing controversy surrounds the CLIA88 regulations, particularly in regard to personnel standards, stringency of quality control requirements, the critical requirement for 'correct' performance in mandated external quality control—proficiency testing—and the role of CLIA88 in physician office laboratories and in the provision of cytology services.

There has been general agreement, Bachner added, on the part of hospitals, professional bodies and the diagnostic manufacturing industry, that the quality control and quality assurance requirements of CLIA88 are overly prescriptive and detailed with considerable potential to impede and discourage the development and introduction of new technologies. An added pressure on practitioners is coming from the immense changes in the financing, organization and delivery of medical and laboratory services currently being implemented in the USA. 'The rapid growth of managed care...has accelerated what many fear to be the deprofessionalization of the practice of medicine and laboratory medicine and is seen as a significant threat to the viability of academic medical centres and medical research.'

Bachner advocates continuing efforts on the part of laboratory professionals and organizations to ensure that professional standards shall be consensual and formulated by professional medical, scientific and laboratory-based organizations. 'Initially, provisional standards should be data-based and referenced to patient-care outcomes as defined by physicians and other clients' of the laboratory, including patients. Final' working standards should be consensual and subject to continual review and modification based upon the ease and practicality of real world' implementation in a wide variety of settings,' he concludes.

New initiatives in the standardization of protein measurements John T. Whicher (Research School of Medicine, University of Leeds, Leeds, UK), Siegfried Baudner (Behringwerke AG, Marburg, Germany), Jacques Bienvenu (Hospices Civils de Lyon, Lyon, France), Soren Blirup-Jensen (Dako A/S, Glostrup, Denmark), Anders Carlstrom (Danderyds Hospital, Danderyd, Sweden), Francesco Dati (Behringwerke AG, Marburg, Germany), Myron A. Johnson (Moses H Cone Memorial Hospital, Greensboro, North Carolina, USA), Robert F. Richie (Foundation for Blood Research, Scarborough, Maine, USA), Per Just Svendsen Dako A/S, Glostrup, Denmark), and Anthony Milford Ward (Protein Reference Unit, Sheffield, UK).

Measurement of the principal human serum proteins has assumed an increasing role in the detection, diagnosis and monitoring of disease and recently certain human serum proteins have also been recognised as useful in the assessment of health. The quantitative measurement and qualitative assessment of a variety of serum proteins can be viewed as a biochemical biopsy that is readily accessible, can be repeatedly inspected, is relatively non-invasive, and can yield useful information much of which in not attainable by other means.

Unlike assays for ions and small molecules, plasma protein measurements depend entirely on comparison of a test sample with a calibrate, known as a reference material or standard. owing to the innate molecular heterogeneity of plasma proteins it is often impossible to ensure that the calibrator is identical in its behaviour in measurement systems to the test sample.

The authors note that a variety of reference materials

for plasma proteins have been in use world-wide over the past 10–15 years. These standards have values assigned in International Units and mass units by several methods against a number of different primary materials. Despite the development in the late 1960s of the World Health Organization's Standards for Immunogloblins in Human Serum and in the late 1970s of the Standard for six Human Serum Proteins, quality control surveys in Western Europe and the United States during the early 1990s showed that values for a given protein may very by as much as 50 to 100%, depending on the reference used.

The solutions to this problem are complex but the use of a single, international reference material by all manufacturers and laboratories has been shown to reduce the variability to a large degree. This has been achieved, the authors note, by the production of a new international reference material for 14 plasma proteins which has been produced by the Community Bureau of References of the Commission of the European Communities (BCR): BCR CRM 470. The project has been managed by the Committee on Plasma Protein Standardisation of International Federation of Clinical Chemistry. The College of American Pathologists (CAP), the major providers of plasma protein reference materials in the USA, have adopted the standard. The material was certified by BCR as a certified reference material (CRM 470) and released jointly with the CAP in mid-1993.

The authors reported that values have been assigned for transthyretin (prealbumin), α_1-acid glycoprotein (orosomucoid), α_1-antitrypsin (α_1-protease inhibitor) and transferrin against new purified protein preparations. Values for albumin, ceruloplasmin, haptoglobin, α_2-macroglobin, C3, C4, IgG, IgA, IgM and C-reactive protein have been assigned against existing international reference materials according to a rigorous protocol designed to test the appropriateness of the candidate preparation as well as the performance of the collaborating laboratories.

A further project, the authors note, has been completed to assign values for α_1-antichymotrypsin and immunoglobulin kappa and lambda light chains. CRM 470 has been released in Europe by BCR and has been approved by the USA Food and Drug Administration for distribution in the USA by CAP. It is available with the protocols and statistical analysis used for the value assignment upon request from BCR, Commission of the European Communities, Directorate General for Science, Research & Development, DG XII/C/5, Measuring & Testing Programme, Rue Montoyer 75, B-1040 Brussels, belgium, and from the College of American Pathologists, 325 Waukegan Road, Northfield, Illinois 60093-2750, USA. It is intended that the material be used as a serum-based reference material for transfer of values to tertiary materials (calibrants and controls) and not for direct use in laboratory assays. It is to be hoped that the use of this common calibrant world-wide for serum protein analysis will result in a demonstrable improvement between laboratories and kits. It is the intention of the committee to assign values for further proteins to the CRM 470 as time and funds will allow.

Other papers presented at the 6th International Congress on Automation and New Technology in Clinical Laboratory, held in Sitges, Barcelona, Spain, 2–4 November 1995, and published in PAC include:

Strategies for immunoassay L. J. Kricka (Department of Pathology and Laboratory Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA).

Micromachining: a new direction for clinical analyzers L. J. Kricka & P. Wilding (Department of Pathology and Laboratory Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA).

Design and implementation of a microchemistry analyzer N. Peled (i-STAT Corp, 303 College Road East, Princeton, NJ 08540, USA).

Neglected aspects in the standardization of protein measurements. A standardized comparison method S, Baudner (Behringwerke AG, BLP—Research Laboratories, PO Box 1140, D-35001, Marburg, Germany).

Practical subminiature immunoanalysis M. A. Johnson (Moses H Cone Memorial Hospital, Greensboro, North Carolina, USA), RF Richie (Foundation for Blood Research, Scarborough, Maine, USA).

Critical aspects in routine coagulation testing A. D'Angelo, P. Della Valle, L. Crippa, E. Pattarini & S. Vigano'D'Angelo (Servizio di Coagulazione, Istitutio Scienitfico HS Raffaele, Via Olgettina 60, 20132 Milano, Italy).

New developments in particle-based immunoassays: introduction L. B. Bangs (Bangs Laboratories Inc, 979 Keystone Way, Carmel, IN 46032-2823, USA).

Determination of β_2-microglobulin in human serum and urine by latex turbidimetry F.-J. Gella & M.-J. Capdevila (Department of Research & Development, Reagents Division, BioSystems SA, Barcelona SA).

Performance of a direct LDL-cholesterol method compared toβ quantification T. Pisani, S. Pickering, L. W. DeLuca & C. P. Gebski (Genzyme Corp, One Kendall Square, Cambridge MA 02139, USA).

The measurement of hormones and bacterial antigens using rapid particle-based immunoassays D. A. Percival (Unipath Ltd, Norse Road, Bedford, MK41 0QG, UK).

Isolation of haematopoietic progenitors. An approach to two different immunomagnetic methods at the lab scale J. A. Cancelas, S. Querol, G. Martin-Henano, C. Canals, C. Azqueta, J. Petriz, J. Esteve-InglCs, B. Amill & J. Garcia (Cryobiology and Cell Therapy Dept, Institut de Recerca Oncolilogica, Barcelona 08907, Spain).

Quantitative reticulocyte counting: Clinical applications I. Cavill (Dept of Haematology, University of Wales College of Medicine, Cardiff, CF4 4XN, UK).

Recent developments in automatic DNA sequencing A. F. Bradley (Perkin-Elmer Hispania SA, Applied Biosystems Division, Ronda de Poniente 5, Tres

Cantos, 28760 Madrid, Spain).

Different approaches to molecular scanning of point mutations in genetic diseases M. Ferrari, P. Carrera & L .Cremonesi (IRCCS, HS Raffaele, Clinical Molecular Biology Laboratory & DBIT, Milan, Italy).

The November 1996, **68**(11), issue of *Pure and Applied Chemistry* is a symposium in print focusing on highlights in the field of bioorganic chemistry. The rapidly growing discipline, which seeks to explore and determine the interaction between organic chemistry and biology, owes much to the development of sophisticated techniques of isolation, detection and structural elucidation of large molecules and molecular systems, including information on the nature of the interactions within such systems. According to the symposium editors, D. St. C. Black (Sydney, Australia), T. Norin (Stockholm, Sweden), and U. K. Pandit (Amsterdam, the Netherlands), the volume presents authoritative articles representative of topics of current interest in the field. The compilation focuses on examples of antibody catalysis, biosynthesis, bioorganic chemistry applied to technology, chemistry and biology of bioactive molecules, and receptors and templates.

The medical potential of catalytic antibodies G. M. Blackburn, A. Datta & L. J. Partridge (Krebs Institute, Department of Chemistry, Sheffield University, Sheffield, UK).

Catalytic antibodies are relatively slow catalysts with turnover numbers some 106 less than is common for enzymes. However, they have the advantage of high affinity for a pre-selected substrate and the ability to carry out a pre-determined chemical transformations with an efficiency that is adequate for medical application. Blackburn *et al.* report two medical targets that readily offer themselves to antibody applications. The first is in the clearance of toxic substances from the blood stream by specific abzyme hydrolysis—such as the hydrolysis of the ester function of cocaine. The second is the conversion of a prodrug into the active agent in a process that is designed to improve either its pharmacokinetic, pharmacological or toxicological profile.

Many groups exploring abzyme-prodrug conversions have focused on ester hydrolyses. However, the *in vivo* application of the approach is hindered because the rate of spontaneous ester hydrolysis is rather high and human serum contains a range of proteins capable of effecting such reactions. Hence the Sheffield group selected carbamate cleavage as the target for prodrug activation and chose to apply it to cancer chemotherapy through the antibody directed enzyme prodrug therapy (ADEPT) concept to try and develop a less immunogenic approach.

ADEPT is a cancer therapeutic programme which builds on the discovery that tumours have specific antigens associated with their surface and that these are

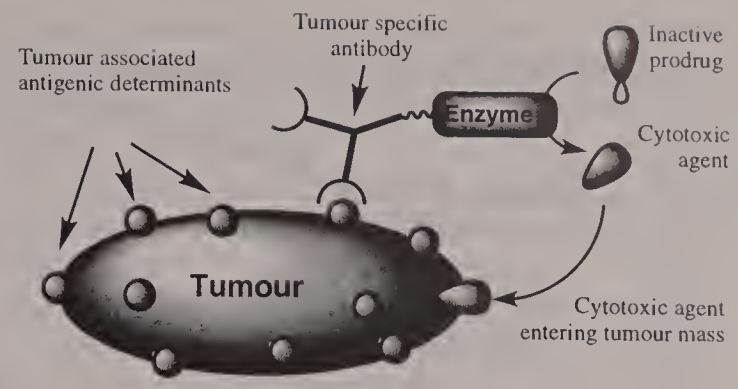


Fig. 2 ADEPT: Mab-enzyme conjugates targeted at the tumour surfaces convert less toxic prodrugs into more active cytotoxic agents.

capable of eliciting an immune response. An effector function, such as an enzyme, can be concentrated in the vicinity of the tumour simply by conjugating it to antibodies which recognise the antibody-specific surface epitopes. Administration of a cytotoxic agent in the form of a prodrug of greatly diminished activity reduces the adverse effects that arise from destruction of fast-dividing, healthy cells in the body. If the effector function, typically an enzyme, can convert the prodrug into the parent cytotoxic agent at the locus of the tumour, then a high concentration of that drug will be delivered selectively to primary and secondary tumour cells.

Problems have been encountered with the ADEPT system, note Blackburn *et al.*, because the enzyme component, usually of bacterial origin, is foreign to the mammalian host and can elicit an immune response. The Sheffield group describes their efforts to get round this problem by developing a non-immunogenic biocatalyst;—a humanisable catalytic antibody, capable of activating a prodrug, a strategy that has been dubbed ADAPT, antibody directed abzyme prodrug therapy. Blackburn *et al.* report how they have obtained several abzymes that not only can generate the desired cytotoxic agent from a prodrug but that they can reduce the viability of a human tumour cell line *in vitro* when incubated with the prodrug.

Nonetheless, the authors caution, some issues remain to be examined further before the full potential of antibodies applied to the target-specific delivery of drugs can be attained. Abzymes remain slow catalysts, they may exhibit slow release of products, the affinity of the monoclonal antibodies for the prodrug is capable of further improvement, and the full integration of pharmacokinetics and pharmacodynamics within the ADAPT systems has to be developed for this approach to reach its full potential *in vivo*.

Genetic selection strategies for generating and characterizing catalysts P. Kast & D. Hilvert (Departments of Chemistry and Molecular Biology, The Scripps Research Institute, La Jolla, CA 92037, USA)

Reengineering of biological macromolecules to elucidate or alter their function is currently one of the most significant research enterprises in modern biological science. Typically, specific positions in a target mol-

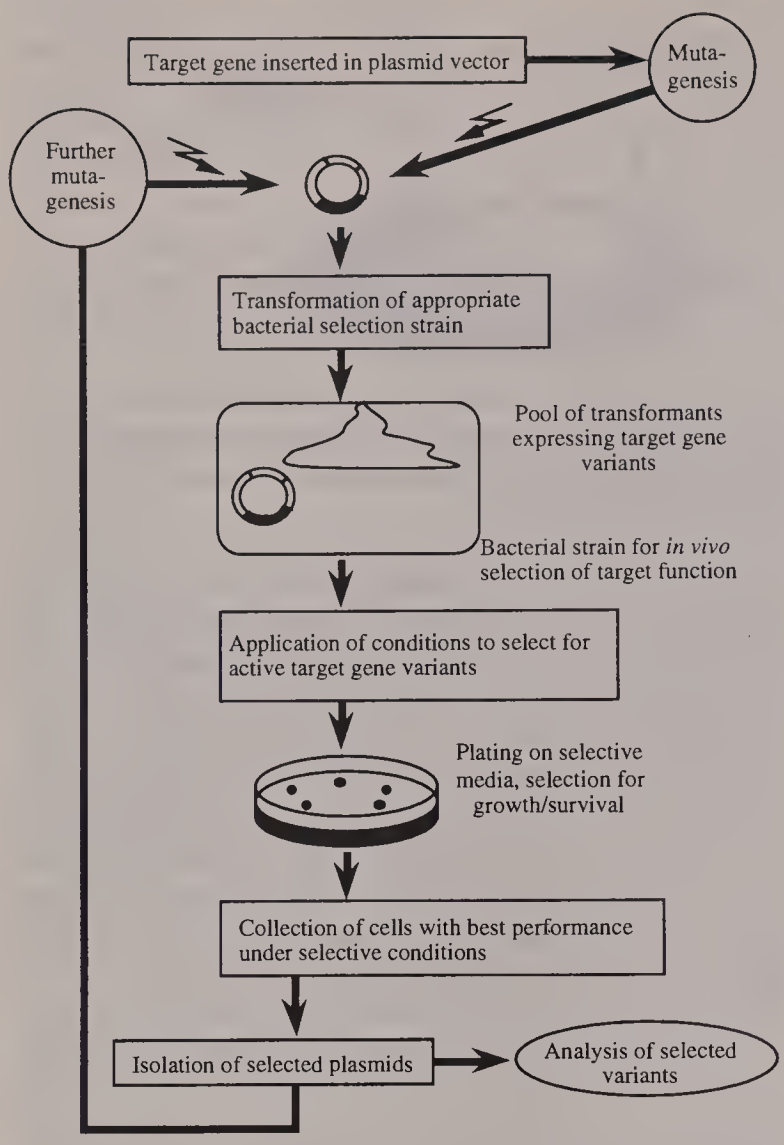

Target gene inserted in plasmid vector
Muta-genesis
Further muta-genesis
Transformation of appropriate bacterial selection strain
Pool of transformants expressing target gene variants
Bacterial strain for *in vivo* selection of target function
Application of conditions to select for active target gene variants
Plating on selective media, selection for growth/survival
Collection of cells with best performance under selective conditions
Isolation of selected plasmids
Analysis of selected variants

Fig. 3 Strategy for catalyst evolution and characterization by random mutagenesis and *in vivo* selection.

ecule, which are assumed to possess functional importance, are modified by site-directed mutagenesis and the effects of the resulting change or changes are assessed. Although this approach is sometimes successful, the so-called 'rational' design frequently fails to yield the expected effect because the complex relationships between sequence, tertiary structure and function may have not been fully elucidated.

Kast & Hilvert believe that molecular evolution is a powerful alternative approach for exploring and creating catalytic function in biological macromolecules. It is an approach which involves random mutagenesis of coding nucleic acids and subsequent selection of individual clones which are capable of performing a desired task. It is well suited to scanning for functional alternatives and creating novel activities in macromolecules such as RNA, DNA and proteins. Kast & Hilvert believe this random approach may prove particularly useful in cases where structural data are not readily available or where mutation is likely to perturb structure.

The authors provide the reader with a general scheme for mutagenesis coupled with selection in vivo which is applicable to enzymes. In it a gene designed to serve as the starting point is cloned into a plasmid vector. this gene is then subjected to randomizing mutagenesis. Depending on the specific case, Kast & Hilvert note, this can be accompanied by a variety of procedures that include chemical mutagenesis, error prone polymer chain reaction, DNA shuffling and degenerate oligonucleotide mutagenesis. The library of resulting plasmid mutants is then introduced into a suitable selection organism, preferable a mutant strain of the well-characterized gut bacterium, *Eschericia coli*. Selective conditions for the desired plasmid-encoded target function are imposed, and growing clones able to satisfy the selection criteria are collected. Finally, analysis of the selected variants yields information about active constellations of amino acid residues. Further rounds of mutagenesis and selection starting from partia

Kast & Hilvert note that there is already a vast collection of examples of the approach. One of the first enzymes to be studied using the methodology was the penicillin and cephalosporin-cleaving TEM-1 beta-lactamase. The results emerging from those investigations have contributed to the understanding of the evolution of clinical antibiotic resistance and have important implications for the design of improved drugs. The approach has also been useful in determining that the catalytic activity of a sluggish mutant triosephosphate isomerase can be partially recovered by second-site amino acid changes.

Genetic selection in a thymidine kinase-deficient *E. coli* strain has been used to identify active clones from random gene libraries encoding variants of herpes simplex virus thymidine kinase, and were used to examine determinants associated with nucleoside binding—a target of antiviral chemotherapy. Among the selected variants, Kast & Hilvert report in their review, were enzymes which phosphorylated thymidine at a higher rate than the wild type, and kinases with altered thermostabilities, and, interestingly with increased activity towards nucleoside analogues such as the antiviral drugs zidovudine, gancyclovir and acyclovir.

Using this approach in their own lab, Kast & Hilvert have been able to find supporting evidence that chorismate mutase—a key reaction in the biosynthesis of the aromatic amino acids phenylalanine and tyrosine in bacteria, fungi and higher plants—has a dipolar active site which is important for catalysis.

Another possibility for the creation of *de novo* catalysts, highlighted by Kast & Hilvert, is the generation of catalytic antibodies. By exploiting the enormous capacity of the mammalian immune system to provide tight binding antibodies to virtually any compound, catalytic immunoglobulins can be elicited with a hapten that mimics the transition states of a desired chemical transformation. An alternative approach for obtaining antibody catalysts makes use of phage display technology for the sampling of large combinatorial libraries composed of immunoselected or unselected immunoglobulin genes

Recent results in pheromone synthesis K. Mori (Department of Chemistry, Faculty of Science, Science University of Tokyo, Kagurazaka 1-3, Shinjuku-ku, Tokyo 162, Japan)

Although bombykol, the first insect pheromone discovered, was an achiral alcohol, many chiral pheromones have since been identified. The importance of the absolute configuration of a chiral pheromone in its expression of bioactivity is now well recognised but owing to the limited amount of natural pheromone available enantioselective syntheses are required both to elucidate the absolute configuration and determine the structure function relationships. Moreover, the asymmetric synthesis of pheromones is of industrial importance as in many cases only one isomer has the desired biological activity while the other invariably inhibits the pheromone action. In this paper, Mori describes new efficient enantioselective syntheses of three insect pheromones: faranal, the trail pheromone of the Pharaoh's Ant; matsuone, the sex pheromone of Matsucoccus Pine Bast Scales; and olean, the sex pheromone of the Olive Fruit Fly. Moreover, as well as reporting the first synthesis of lurlene, the sex pheromone of the green flagellate Chlamydomonas allensworthii, Mori also describes the synthesis of a fluorinated analogue of blattellastanoside A, the aggregation pheromone of the German cockroach, which is biologically more potent than the natural compound.

Template assisted protein *de novo* design G. Tuchscherer & M. Mutter (Institute of Organic Chemistry, University of Lausanne, BCH-Dorigny, CH-1015, Lausanne, Switzerland)

The ultimate goal in protein *de novo* design is the construction of artificial proteins exhibiting tailor-made structural and functional properties. Yet, as Tuchscherer & Mutter report, creating native-like macromolecules by copying Nature's way has proven to be difficult because the mechanism of folding in its complexity has still to be unravelled. In the absence of a detailed knowledge of the folding mechanism of natural proteins a general design strategy of polypeptide sequences with a high propensity to fold in a pre-determined three dimensional structure appears still out of reach. There are currently two basic hypotheses on the problem of protein folding mechanisms. One is based on the assumption that folding is initiated by the formation of fluctuating elements of local secondary structure along the unfolded polypeptide chain; subsequent interactions between these ordered regions and simultaneous rearrangements apparently lead to the formation of a compact globular structure. Alternatively, it is postulated that the unfolded polypeptide chain first collapses into a fairly compact 'molten globule' state followed by the formation of specific secondary structures. These hypotheses are not mutually exclusive and could be reconciled to a unified theory on protein folding.

In this review, Tuchscherer & Mutter describe a con-

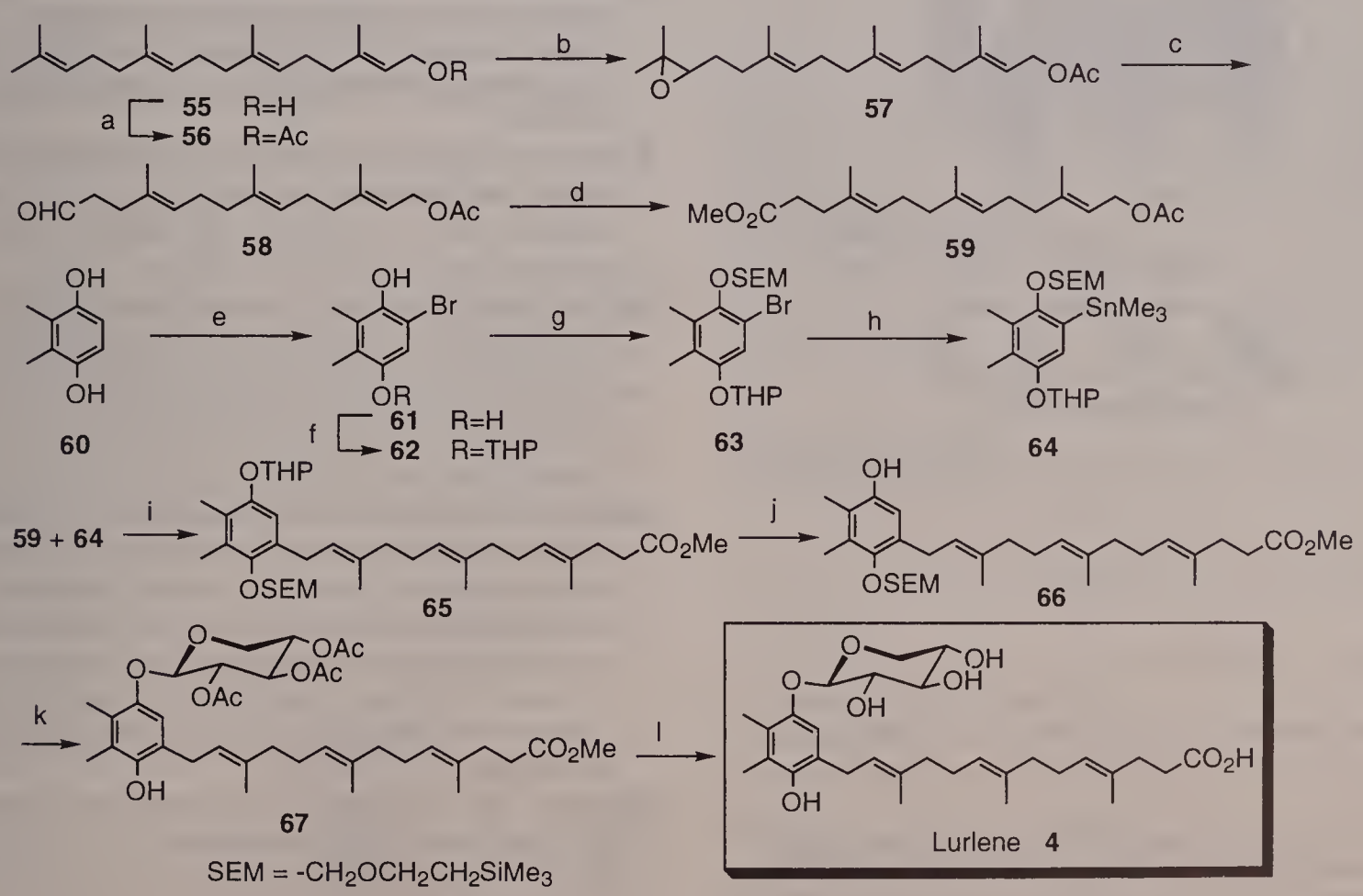


Fig. 4 Synthesis of lurlene.

ceptually different approach in protein design, the concept of template assembled synthetic proteins (TASP), to bypass the folding problem. The authors argue that topological templates as 'built-in' devices for the induction of well-defined folding topologies and progress in synthetic strategies—such as chemoselective ligation methods and the use of pseudoprolines to enhance peptide solvation—open the way for the design of more complex, and hence functional TASP molecules.

Peptide chemists are no longer bound to copy Nature's way of peptide synthesis and protein folding. With progress in the synthetic strategy and structural characterization of this new type of macromolecule, Tuchscherer & Mutter contend that chemists are now one step closer to mimicking more realistically some functional properties of natural proteins such as vaccines, catalysts and ion channels or even to combine different independent folding topologies which at the same time resemble different functionalities.

Other papers published in the PAC Symposium in Print 'Highlights in Bioorganic Chemistry' include:

Catalytic antibodies: Regio- and enantioselectivity in a hetero Diels–Alder reaction M. Resmini, A. A. P. Meekel & U. K. Pandit (Laboratory of Organic Chemistry, University of Amsterdam, Nieuwe Achtergracht 129, 1018 WS, Amsterdam, the Netherlands)

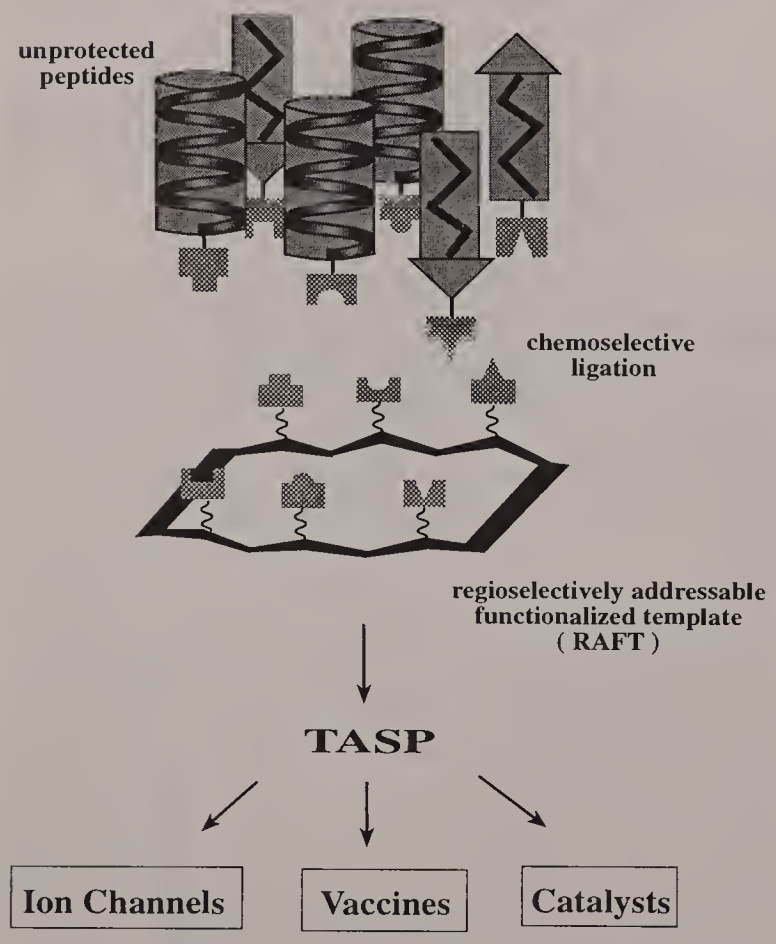


Fig. 5 The use of unprotected peptide segments and selectively addressable templates in chemoselective ligation procedures allows for the construction of more complex TASP molecules resembling ion channels, catalyst or vaccines.

The transformylase enzymes of *de novo* purine biosynthesis M. S. Warren, K. M. Mattia, A. E. Marolewski & S. J. Benkovic (The Pennsylvania State University, Department of Chemistry, 152 Davey Laboratory, University Park, PA 16802, USA)

Why natural DNA is based on 2′-deoxyribose, with 3′-5′ phosphodiester links R. Breslow & T. L. Sheppard (Department of Chemistry, Columbia University, New York, NY 10027, USA)

Chiral chemodiversity and its role for biological activity. Some observations from studies on insect/insect and insect/plant relationships T. Norin (Department of Chemistry, Organic Chemistry, Royal Institute of Technology, S-10044 Stockholm, Sweden)

Biomimetic syntheses of alkaloids based on tetrahydropyridine M. J. Wanner & G. J. Koomen (Amsterdam Institute of Molecular Studies. Laboratory of Organic Chemistry, University of Amsterdam, Nieuwe Achtergracht 129, 1018 WS, Amsterdam, the Netherlands)

Vitamin B_{12}. Recent discoveries cast new light on an ancient structure A. I. Scott (Department of Chemistry, Texas A&M University, College Station, Texas 77843-3255, USA)

Stereochemical aspects of flavour biogeneration through baker's yeast mediated reduction of carbonyl-activated double bonds G. Fronza, C. Fuganti, M. Mendozza, R. Rigoni, S. Servi & G. Zucchi (Dipartimento di Chimica del Politecnico, CNR Centro di Studio per le Sostanze Organiche Naturali, Via Mancinelli 7, 20121 Milano, Italy)

Plant cell culture combined with chemistry—a powerful route to complex natural products J. P. Kutney (Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver BC, Canada V6T 1Z1)

A chemoenzymatic approach to carbohydrate-mediated cell adhesion M. Hendrix & C.-H. Wong (Department of Chemistry, The Scripps Research Institute, La Jolla, CA 92037, USA)

On the interaction of lignin peroxidase with lignin H. E. Schoemaker (Laboratory of Organic Chemistry, University of Amsterdam, Nieuwe Achtergracht 129, 1018 WS, Amsterdam, the Netherlands) & K. Piontek (ETH-Zurich, Laboratory of Biochemistry I, Universitatstrasse 16, CH-8092, Zurich, Switzerland)

Bacterial 2-haloacid dehalogenases: Structures and catalytic properties K. Soda, T. Kurihara, J.-Q. Liu, V. Nardi-Dei, C. Park & N. Esaki (Laboratory of Microbial Biochemistry, Institute for Chemical Research, Kyoto University, Uji, Kyoto 611, Japan) and M. Miyagi & S. Tsunasawa (Biotechnology Research Laboratories, Takara Shuzo Co Ltd, Otsu, Shiga 520-21, Japan)

Structure and function of the potassium channel inhibitor from black scorpion venom E. V. Grishin, Yu V. Korolkova, S. A. Kozlov, A. V. Lipkin, E. D. Nosyreva, K. A. Pluzhnikov, S. V. Sukhanov & T. M. Volkova (Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences,

ul. Miklukho-Maklaya, 16/10, 117871, GSP-7, Moscow, Russia)

Use of carbohydrates and peptides in studies of adhesion of pathogenic bacteria and in efforts to generate carbohydrate-specific T cells J. Kihlberg & G. Magnusson (Organic Chemistry 2, Chemical Center, The Lund Institute of Technology, Lund UNiversity PO Box 124, S-221 00 Lund, Sweden)

Chemistry and biology of selected natural products K. C. Nicolaou, E. A. Theodorakis & C. F. Claiborne (Department of Chemistry, The Scripps Research Institute, La Jolla, CA 92037, USA, and Department of Chemistry and Biochemistry, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093, USA)

How do the energetics of the stereoelectronic gauche and anomeric effects modulate the conformation of nucleos(t)ides? J. Plavec, C. Thibaudeau & J. Chattopadhyaya (Department of Bioorganic Chemistry, Box 581, Biomedical Centre, Uppsala University, S-751 23 Uppsala, Sweden)

Templates, autocatalysis and molecular replication B. G Bag (Department of Organic Chemistry, Indian Institute of Science, Bangalore, India) & G. von Kiedrowski (Institute of Organic Chemistry and Biochemistry, Albert Ludwig University, Freiburg, Germany)

Development of supramolecular metalloprotein mimics M. C. Feiters, R. J. M. Klein Gebbink, A. P. H. J. Schenning, G. P. F. van Strijdonck, C. F. Martens & R. J. M. Nolte (Department of Organic Chemistry, NSR Centre, University of Nijmegen, Toernooiveld, 6525 ED Nijmergen, the Netherlands)

Effects of crown ethers and small amounts of cosolvent on the activity and enantioselectivity of alpha-chymotrypsin in organic solvents J. F. J. Engbersen, J. Broos, W Verboom & D. N. Reinhoudt (Department of organic Chemistry, Faculty of Chemical Technology, University of Twente, PO Box 217, 7500 ARE Enschede, the Netherlands)

Screening of boronic acids for strong inhibition of the hydrolytic activity of alpha chymotrypsin and for sugar sensing associated with a large fluorescence change H. Suenaga, H. Yamamoto & S. Shinkai (CHEMIRECOGNICS project, ERATO, Research Department Corporation of Japan, 2432-3 Aikawa-cho, Kurume, Fukuoka 830, Japan)

Structural reporter parameters for the characterisation of crystalline cellulose A. P. Heiner & O. Teleman (Biotechnology and Food Research, VTT Technical Research Centre of Finland POB 1500, FIN-02044 VTT (Espoo), Finland).

News

FECS General Assembly details future plans

General Assembly

The General Assembly of the Federation of European Chemical Societies met in Athens on 19–20 September as the guest of the Association of Greek Chemists. Local arrangements were made by Dr N. Katsaros. Representative of 20 member societies participated, together with chairmen of the FECS divisions and working parties. Dr E. D. Becker, secretary general of IUPAC, also participated. Professor L. Niinisto (Association of Finnish Chemical Societies), the President of FECS, chaired the meeting. The Ukrainian Chemical Society was admitted to membership.

A powerful voice for chemists

The FECS General Assembly voted *nem. con.* to adopt the new constitution, thus confirming the cooperation between ECCC (European Communities Chemistry Council) and FECS and creating an organization which will act as a powerful single voice for chemists and chemistry in Europe. The new organization has significant resources to call upon, having over 40 member societies which, in total, represent some 200 000 individual chemists in academia, industry and government in 32 countries across Europe.

The constitution requires FECS, as a non-profit-making organization, to promote the advancement of chemical sciences and the practice of chemistry in Europe, taking account of issues of particular relevance to the European Union. FECS will therefore:

- promote effective communication throughout the community of chemists in Europe;
- promote collaborative activity among member societies and among the individual members of these societies;
- maintain and promote high professional, educational and ethical standards;
- disseminate chemical knowledge;
- maintain a policy of safeguarding the environment;
- act in an advisory, consultative and representative capacity in relation to European institutions.

Scientific meetings, sponsored events and development of initiatives in specific areas are carried out by divisions and working parties. The restructured organi-

zation will develop further the ECCC expertise in educational and research matters, for example the designation European Chemist and the AllChemE initiative. FECS is keen to expand collaborative activity with other organizations, including CEFIC and the European Federation of Chemical Engineers (ECFE). The EUCHEM Committee, which organizes high level scientific conferences, is an integral part of FECS.

The designation European Chemist

Participation in the European Chemist Registration Board, the awarding body for European Chemist (EurChem) is no longer restricted to EU countries—it is open to all FECS member societies across Europe who can fulfil the criteria for being a responsible body for assessing the qualifications of their members. A prerequisite is that the appropriate academic qualifications from the country concerned should be listed in the ECCC schedule of category-A qualifications.

FECS Executive

A new executive committee will oversee the scientific, educational and professional activities of FECS: Professor L. Niinisto (President) (Finland), Dr P. B. Czedik-Eysenberg (Austria), Professor J.-B. Donnet (France), Dr T. D. Inch (UK), Professor N. Z. Lyakhov (Russia), Professor G. Naray-Szaba (Hungary), Professor J. A. Rodriguez Renuncio (Spain), Professor H. tom Dieck (Germany), Professor B. Stanovnik (Slovenia), together with the chairmen of the divisions.

Divisional activities

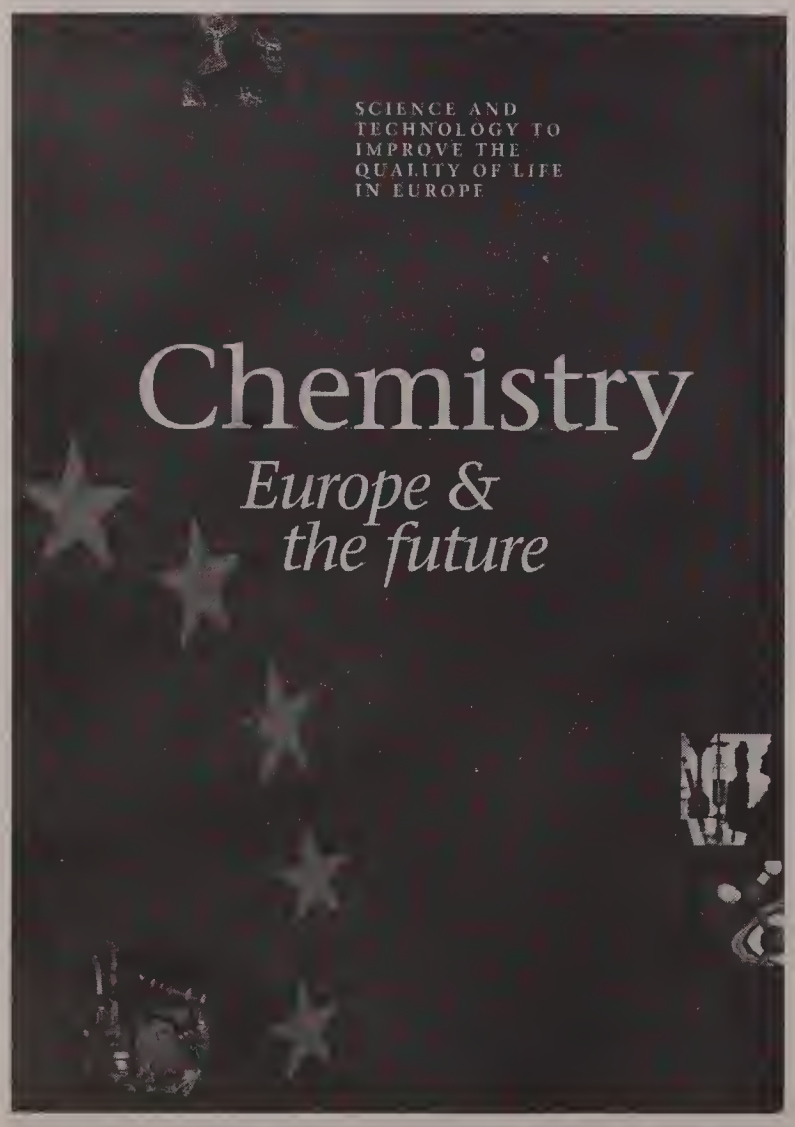
The principal activities of FECS have been undertaken by its ten working parties. In order to enhance some of this activity, FECS has converted three of the working parties into divisions:

- Division of Analytical Chemistry, chaired by Professor R. Kellner (Austria);
- Division of Food Chemistry, chaired by Dr R. Battaglia (Switzerland);
- Division of Chemistry and Education, chaired by Dr J. M. F. Gagan (UK).

and is considering the future status of the others. A task group is looking at potential new areas of divisional activity for FECS, including any interdisciplinary areas that should be seen to have a European dimension.

Each division organizes a European conference every two years, for example Euroanalysis (in Basel in 1998), ECRICE—Research in Chemical Education (in York in September 1997), and EuroFoodChem (in Interlaken in September 1997).

Following the success of its Eurocurriculum on Analytical Chemistry, the division of Analytical Chemistry is publishing an International Undergraduate Textbook based on the Eurocurriculum. The division of Food Chemistry is developing a Eurocurriculum in Food Chemistry.



FECS Award

The FECS Award for 1996 was presented by the President to Professor Ferenc Szabadvary (Hungarian Chemical Society), chairman of the working party on the history of chemistry for many years, for his very valuable contribution to the work of FECS. The working party on history of chemistry has produced a Guide of European Museums with collections on the History of Chemistry. The 127 page guide costs USD8.00 and is available from FECS.

Chemists call for European policy for science and technology AllChemE, an alliance of five organization representing chemists, chemical engineers and technologists in Europe, is calling on Europe's politicians to support the chemical industry. In the foreword of a report 'Chemistry: Europe and the Future', Nobel Laureates Richard Ernst, Jean-Marie Lehn and Lord Lewis of Newnham FRS, joined with Simon de Bree, president of Cefic, the European Chemical Industry Council, to warn that the future prosperity of Europe depends on the European chemical industry remaining competitive in the global marketplace. The current trend of companies shifting many of their activities outside Europe, how-

ever, could precipitate a downward spiral of less innovation, less creativity, and ultimately, a loss of quality of life in Europe.

'The European chemical industry is an outstandingly successful industry that contributes Ecu30bn to Europe's trade balance and employs 1.65 million people. There are also many industries such as agriculture, car manufacturers, which rely heavily on the chemical industry,' notes Jon McCleverty, professor of inorganic chemistry at the University of Bristol and Chairman of CERC3—chairmen of the European Research Councils Chemistry Committees. 'If the chemical industry disappeared tomorrow, it would be the equivalent of putting the population of a medium-sized European county out of work. Industry is reliant on universities for its workforce so we must ensure that academic institution are properly funded.'

The authors of the report argue that the chemical industry is one of the foundations of the European community noting that 150 years of fruitful interaction between academics and industry has led to impressive economic strength. And while the chemical industry is currently performing well and making significant contributions to the economies of Europe, there are clouds on the horizon. 'It is possible that in 15–20 years' time, unless action is taken now, Europe may be importing what it once had no difficulty in producing and we may be paying patent royalties on what we might otherwise have invented ourselves. We will then see our brightest young scientists leaving to work elsewhere, reversing the tradition of Europe attracting young chemists from around the world.'

Professional affairs

For many years there has been an FECS working party acting as a forum for those societies that wished to discuss professional affairs. Some of the activity has been associated with the activities of the ECCC. The FECS Council has proposed that, under the new integrated structure, issues of professional affairs of interest to the FECS societies, for example manpower statistics, should be handled under the auspices of ECCC.

Further information on FECS/ECCC is available on the internet at http://chemistry.rsc.org/rsc/fecs.htm and http://chemistry.rsc.org/rsc/eccc.htm or from Ms E. K. McEwan at the RSC, email: mcewane@rsc.org

IUPAC colleagues deceased

We have been informed of the death of IUPAC colleagues:

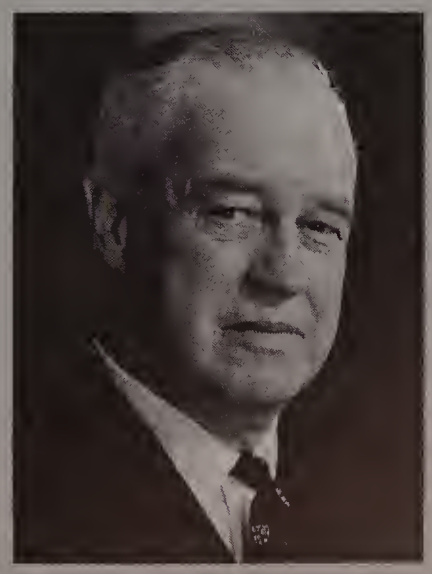
New Zealand: Dr T.A. Rafter (26 September 1996)—Commission on Radiochemistry and Nuclear Techniques (1971–1981).

Russia: Prof. V.A. Koptyug (10 January 1997)—President of IUPAC (1987–1989), Commission on Molecular Structure and Spectroscopy (1975–1983), Coordinating Committee on Chemistry and Environment Programme (1989–1993).

UK: Prof. R.M. Barrer (12 September 1996)—Commission on Colloid and Surface Chemistry including Catalysis (1969–1977).

Lord (Prof. Alexander) Todd (10 January 1997)—President of IUPAC (1963–1965), Vice-President of Organic Chemistry Division (1957–1959)/ Member of Division Committee (1955–1957), Editorial Board (1959–1965), Coordinating Committee for Analytical Methods for CEE and IARC (1966–1969).

Prof. V.A. Koptyug (USSR) 1987–1989.



Lord Todd (UK) 1963–1965.

Names and addresses

Full details (names, addresses, telephone/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* 1995, **17**(6), 212–226. The IUPAC Secretariat has been notified of the following changes:

Prof. E. Baciocchi (Secretary, Commission III.2), Dipartimento di Chimica, Universita 'La Sapienza' Piazzzale Aldo Moro 5, I-00185 Roma, Italy.

Dr B. Heinzow (Secretary, Commission VII.C.2), Landesamt fur Natur und Unwelt des Landes Schleswig-Holstein, Hamburger Chaussee 25, D-24220 Flintbek, Federal Republic of Germany; Tel.: +49 4347 704 200; Fax: +49 4347 704 202; E-mail: heinzow@t-online.de

Dr W.H. Koppenol (Secretary, Commission II.2), E-mail: willem.koppenol@inorg.chem.ethz.ch

Dr A. Marton (Chairman, Commission V.3), Fax: +36 88 421 869.

Dr D.R. Moore (Chairman, Commission IV.2), E-mail: roy.moore@wilton.ici.co.uk

Prof. J. Ralston (Chairman, Commission I.6), Tel.: +61 8 8302 3066; Fax: +61 8 8302 3683; E-mail: john.ralston@unisa.edu.au. Prof. M. Quack (Secretary, Commission I.1), E-mail: quack@ir.phys.chem.ethz.ch

Dr T.R. Roberts (Secretary, Chemistry and the Environment Division), JSC International Ltd, Osborne House, 2- Victoria Avenue, Harrogate, North Yorkshire HG4 3QL, UK.

Prof. J.G. Traynham (Secretary, Commission III.1), 628 Polytech Drive, Baton Rouge, Louisiana 70808-4755, USA; Tel.: +1 504 766 2163.

Recent reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry*.

Nomenclature of carbohydrates (IUPAC Recommendations 1996)

These Recommendations expand and replace the Tentative Rules for carbohydrate Nomenclature issued in 1969 jointly by the IUPAC Commission on the Nomenclature or Organic Chemistry and the IUB-IUPAC Commission on Biochemical Nomenclature (CBN). They also replace other published JCBN Recommendations that deal with specialized areas of carbohydrate terminology. The present Recommendations deal with the acyclic and cyclic forms of monosaccharides and their simple derivatives, as well as with the nomenclature of oligosaccharides and polysaccharides. They are additional to the Definitive Rules for the Nomenclature of Organic Chemistry and are intended to govern those aspects of the nomenclature of carbohydrates not covered by those rules. Carbohydrate nomenclature has a fairly rich history, the Commission notes in its preamble. In the early nineteenth century, individual sugars were often named after their source, such as grape sugar (traubenzucker) for glucose, and cane sugar (rohrzucker) for saccharose (later dubbed sucrose). The name glucose was first coined in 1938 while Kekule proposed the name dextrose in 1866 because glucose is dextrorotatary. Similarly, the laevorotatory fruit sugar (fruchtzucker or fructose) was for a time dubbed laevulose. A consensus rapidly emerged supporting the use of the -ose suffix for sugars. The term carbohydrate was applied originally to monosaccharides, in recognition of the fact that their empirical composition can be expressed as $C_n(H_2O)_n$. Based on the fundamental researches of Emil Fischer and others in the 1880s, the JCBN notes that the foundations of terminologies were laid down, based on the terms triose, tetrose, pentose and hexose. Taking into account the developing concept of stereochemistry, Fischer introduced the now classical projection formulae for sugars, with a standard orientation viz. carbon chain vertical, carbonyl group at the top. Fischer assigned to the dextrorotatary glucose (via the derived glucaric acid) the projection with the OH group at C-5 pointing to the right, well knowing that there was a 50% chance that he was wrong, which he was not. In 1906,

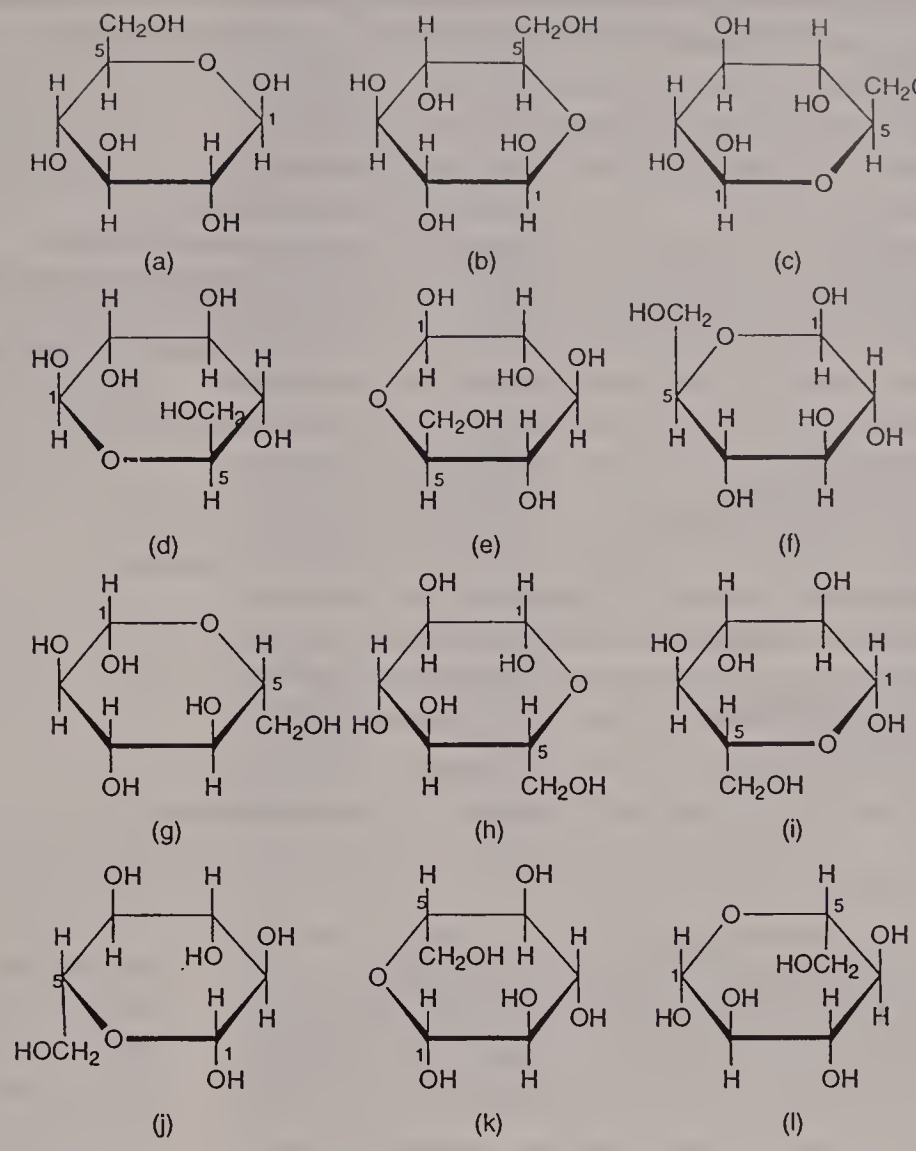


Fig. 1 β-D-Glucopyanose in the twelve possible Haworth representations (the hydrogen atoms are frequently omitted).

Rosanoff selected the enantiomeric glyceraldehydes as the point of reference; any sugar derivable by chain lengthening from what is now known as D-glyceraldehyde belongs to the D series, a convention still in use.

Towards the end of the nineteenth century it was realized that the free sugars existed as cyclic hemiacetals or hemiketals. Mutorotation was interpreted as being due to a change in the configuration of the glycosidic (anomeric) carbon atom. Fischer assumed the cyclic form to be a five membered ring which Tollens designated by the symbol <1,4>, while the six-membered ring received the symbol <1,5>. Haworth and his school, in the 1920s, proposed the terms 'furanose' and 'pyranose' for the two forms. Haworth also introduced the 'Haworth depiction' for writing structural formulae, a convention that was soon widely followed.

Up to the 1940s, nomenclature proposals were still very much made by individuals. Official bodies such as the International Union of Chemistry, although developing and expanding the Geneva nomenclature for organic compounds, made little progress with carbohydrate nomenclature. The IUPAC Commission on Nomenclature of Biological chemistry out forward a classification scheme for carbohydrates, but the new terms proposed have not survived. However, in 1939 the American Chemicals Society (ACS) formed a committee to look into this matter, since rapid progress in the field had led to various misnomers arising from a lack of guidelines. Thus the foundations of modern systematic nomenclature for carbohydrates and derivatives were laid: numbering of the sugar chain, the use of D and L and alpha and , and the designation of stereochemistry by italicized prefixes. The final report was approved and published by the ACS in 1948.

However, not all problems were solved, and to cope with the differing usages encountered on either side of the Atlantic a joint British-American committee was established. In 1952 that committee published 'Rules for Carbohydrate Nomenclature'. That work was continued, resulting in the endorsement and publication of a revised version in 1963 by the ACS and the Chemical Society of Britain. That prompted the IUPAC Commission on Nomenclature of Organic Chemistry to consider preparation of a set of IUPAC Rules for Carbohydrate Nomenclature, which was conducted jointly with the IUPAC-IUB Commission of Biochemical Nomenclature, and resulted in the 'Tentative Rules for Carbohydrate Nomenclature, Part I, 1969', published in 1971/72 in several journals. The Joint Commission of Biochemical Nomenclature has now published in PAC a revision of that 1971 document.

Table 1 Symbols for monosaccharide residues and derivatives in oligosaccharide chains

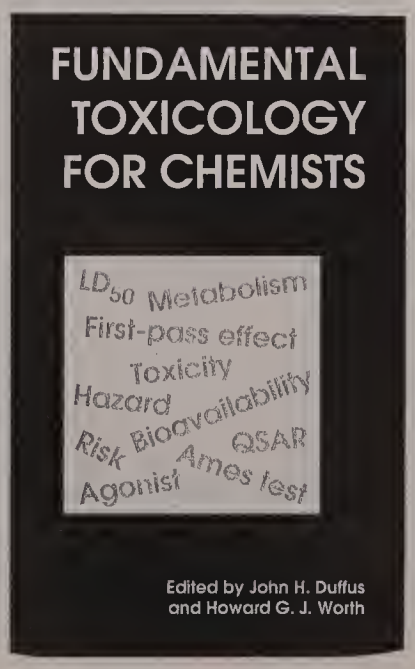
Abequose	Abe	Iduronic acid	IdoA
Allose	All	Lyxose	Lyx
Altrose	Alt	Mannose	Man
Apiose	Api	Muramic acid	Mur
Arabinose	Ara	Neuraminic acid	Neu
Arabinitol	Ara-ol	*N*-Acetyineuraminic acid	Neu5Ac
2-Deoxyribose	dRib	*N*-Acetyl-2-deoxyneur-2-enaminic acid	Neu2en5Ac
Fructose	Fru	*N*-Glycoloyineuraminic acid	Neu5Gc
Fucose	Fuc	3-Deoxy-D-*manno*-oct-2-ulosonic acid	Kdo
Fucitol	Fuc-ol	Rhamnose	Rha
Galactose	Gal	3,4-Di-Gmethylrhamnose	Rha3,4Me_2
Galactosamine	GalN	Psicose	Psi
N-Acetylgalactosamine	GalNAc	Quinovose	Qui
β-D-Galactopyranose 4-sulfate	β-D-Gal*p*4S	Ribose	Rib
Glucose	Glc	Ribose 5-phosphate	Rib5*P*
Glucosamine	GlcN	Ribulose	Ribulo (or Rul)
2,3-Diamino-2,3-dideoxy-D-glucose	GlcN3N	Sorbose	Sor
Glucitol	Glc-ol	Tagatose	Tag
N-Acetylglucosamine	GlcNAc	Talose	Tal
Glucuronic acid	GlcA	Xylose	Xyl
Ethyl glucopyranuronate	Glc*p*A6Et	Xylulose	Xylulo (or Xul)
Gulose	Gul	2-*C*-Methylxylose	Xyl2*C*Me
Idose	Ido		

This report was prepared for publication by A. D. McNaught (The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF, UK) for the Joint Commission on Biochemical Nomenclature of IUPAC and the International Union of Biochemistry and Molecular Biology. The full details are to be found in Pure Appl. Chem. *1996,* ***68****, 1919–2008.*

New publications

Fundamental toxicology for chemists

There is an increasing awareness throughout the world of safety and a consciousness of the need for safety standards. This has occurred not least in chemistry and the handling of chemicals, and is not confined to the laboratory. Chemicals are increasingly being used in domestic and non-technical environments where their safe handling is no longer solely the concern of qualified chemists. For instance, the use of domestic cleaners, solvents and detergents, weed killers and pesticides, and proprietary medicines. Many of these are powerful and dangerous chemicals, particularly in the hands of those who do not understand the implication of their actions. Many countries have passed legislation concerned with practices in the workplace. This has been led by the countries of Europe and North America and other developed nations, but it is spreading and will spread throughout all areas of the world.



In 1974, the UK passed the Health & Safety at Work Act, which required the appointment of safety representatives, the establishment of safety committees, and the inspection of the workplace by representative and/or members of the safety committee. This had implications for the handling of chemicals where these are used in the workplace. More recently, regulations for the Control of Substances Hazardous to Health (COSHH) require laboratories and institutions to compile and retain inventories of chemicals used within their laboratories. The inventory must include statements concerning toxic properties, handling procedures, and actions that should be taken in the event of

Proposed timetable for curriculum of fundamental toxicology for chemists

Section 1 Introduction to toxicology	12h
Hazard, toxicity and fundamental concepts. Toxicity testing and epidemiology as sources of information Toxicokinetics Exposure, adsorption, distribution, storage, metabolism, and excretion Toxicodynamics Fundamental mode of action of toxicants in causing harmful effects	
Section 2 Application of toxicity data	8h
Toxicity data interpretation Risk assessment and risk management Monitoring exposure	
Section 3 Specialized aspects of toxicology	8h
Mutagenicity Carcinogenicity Reproductive toxicity Immunotoxicity	
Section 4 Organ toxicology	10h
Skin toxicology Respiratory toxicology Hepatotoxicity Nephrotoxicity Neurotoxicity	
Section 5 Complex aspects of toxicology	5h
Behavioural toxicology Ecotoxicity	
Section 6 Special toxicants	4h
Radionuclides Biocides	
Section 7 Safe handling of chemicals	2h
Summary and review	1h
Total	50h

an accident or spillage. The safe handling of potentially toxic biological materials has been dealt with in the UK by the Department of Health and Social Security, which has produced a series of documents culminating in 'Code of Practice for the Prevention of Infection in Clinical Laboratories and Postmortem Rooms'. This document was produced at the international level, the International Programme on Chemical Safety, a joint activity of the World Health Organization, the United Nations Environmental Programme and the International Labour Organization, produces international chemical safety cards in conjunction with the Commission of the European Communities. This is only one example of such activity through international bodies. As the output of such international bodies increases, so will national recognition of the need for chemical safety throughout the world. These activities are happening in tandem with legislation and the establishment of standards for the safe disposal of chemicals. Intrinsic to all this activity are the concepts of risk assessment and risk management particularly in the context of industrial chemical processes.

It seems reasonable that chemists should be aware of these dangers within their laboratories and that there should be documentation and legislation to help the safety process. It has already been intimated that this not confined to the laboratory, as chemicals are used increasingly in the domestic and non-technical environment, where their safe handling is no longer the sole concern of qualified chemists. The question is asked, therefore, who is the person to whom the public might turn to seek advice and help in the safe handling of chemicals. More often than not the answer that comes back is the chemist, and it is not unreasonable that the chemist is seen as the person that can give help and advice on the handling of chemicals, on the toxic effects associated with them, on how to deal with an incident if and when it occurs, and to have some understanding of the risk management and environmental issues involved in handling chemicals on a larger scale.

Unfortunately, this is not recognised formally in the curricula of the training of the majority of chemists. Indeed, apart from what they pick up incidentally as part of their education progress, there is often no formal training in the teaching of toxicology. This makes chemists very vulnerable now that the legal responsibilities of risk assessment make them liable to large claims for damages, especially at the level of responsible management. The problem has been addressed by IUPAC through a joint project involving IUPAC's Commission on Toxicology and its Committee on Teaching of Chemistry. This collaboration has been able to call upon expertise in both toxicology and teaching. The project aimed at producing a text book for the chemistry teachers and students on basic selected topics which cover those areas of toxicology which are most related to the requirements of chemists, as follows:

- Toxicokinetics and toxicodynamics
- Data interpretation
- Risk assessment and management
- Exposure and monitoring
- Mutagenicity
- Carcinogenicity
- Reproductive toxicity
- Immunology and immunotoxicity
- Skin toxicity
- Respiratory toxicity
- Hepatotoxicity
- Nephrotoxicity
- Neurotoxicity
- Behavioural toxicity

- Ecotoxicity
- Radionuclides
- Biocides and pesticides
- The safe handling of chemicals

As this book is aimed at teachers as well as students, it includes proposals for a curriculum based on 50 hours teaching.

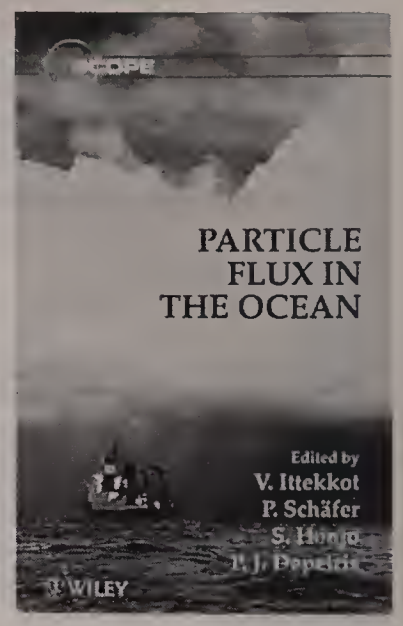
Through the varied knowledge and expertise of the members of the IUPAC Toxicology Commission, it has been possible to invite authors, who are recognised experts in their own areas, to contribute to the book. The teaching expertise of the Commission on Teaching of Chemistry means that the whole book has been appraised at the draft stage by experts in teaching, including those whose prime concern is tertiary teaching. We believe that this has given IUPAC a unique opportunity to produce a publication on those aspects of toxicology which are fundamental for the qualified chemist. Moreover, it addresses the requirements of teacher and student alike, and which we hope will form the basis of an essential curriculum for future modular university programmes in chemistry throughout the world, reflecting the increasing necessity for chemists to understand the basics of toxicology and its implications.

Fundamental Toxicology for Chemists is published by the Royal Society of Chemistry, ISBN 0 85404 529 5, price GBP29.50.

Hrvatska nomenkaltura anorganske kemije

A Croatian translation of the *Red Book (1990), Nomenclature of Inorganic Chemistry*, has recently been published by the Croatian Chemical Society. The original text has been adapted and translated by Professor Bozidar Grabaric, Dr August Janekovic, Dr Milenko Markovic, Dr Vera Simeon-Rudolf, Professor Hrvoj Vancik and Profesor Vladimir Simeon, all of the University of Zagreb. Professor Simeon also edited the whole text. The translation has been officiak recommended by the Croatian Chemical Society. Anyone interested in obtaining a copy of this Croatian translation of the Red Book should contact Professor Simeon, Chemistry Department, Faculty of Science & Mathematics, University of Zagreb, Marulicev trg 19/11, HR-10001, Zagreb, POB 163, Croatia.

Particle Flux in the Ocean



The global balance of water, carbon dioxide and radiation regulate the climate of our planet. The involved fluxes of matter and energy are conditioned by the pressure of life on Earth. Hence, it it the existence of living organisms—unicellular in the first place—to whom the Earth's surface owes its shape a and habitability. Biogeochemical element cycles are a manifestation of the permanent material exchange between the living and the non-living world. There is variability in the fluxes on a continuous spectrum of space and time scales covering several orders of magnitude. In this context, particle flux in the ocean is a unique phenomenon in that it encompasses a wealth of mechanisms that operate on the whole range of space and time scales, that involve innumerable interactions between the living and the non-living world and provide a link between the ocean-atmosphere boundary, the deep sea and the sediments. Its relevance on the climate system ranges from the seasonal cycle of pCO_2 to the deposition of sediment on geologic timescales.

The papers in *SCOPE 57: Particle Flux in the Ocean* provide information collected over several years by scientists world-wide which will eventually provide the answer. The pattern that emerges is that particle flux in the ocean responds to many geophysical parameters: Wind speeds and aerosol

deposition over the oceans, nutrient levels, CO_2 levels in the mixed layer, the availability of trace elements such as iron, and volcanic emissions, all affect particle flux in the oceans. Many of the parameters have been anthropogenically perturbed. Thus the present particle flux measurements—even in the open ocean areas—must no longer give natural background values.

Since fertilizer, CO_2 and trace element input to the sea have increased, one is tempted to claim a particle flux increase in the ocean as well, but this would be a premature statement. Some of the basic questions therefore are: Is particle flux in the ocean on a secular steady state or anthropogenically perturbed? Would the perturbation influence the long For more than a decade the SCOPE/UNEP Carbon Unit at the Hamburg University has initiated and coordinated projects on the Global Carbon Cycle.

Publication of this volume brings to a close a phase of the Global Carbon Cycle project which has concentrated on understanding the flow, interaction and fate of carbon and other nutrients from land via rivers to lakes and to deep oceans. It is also the outcome of the final workshop on Particle Flux in the Ocean, which was held in Hamburg, Germany in September 1993. Scientists from several countries, including Argentina, Brazil, Chile, the People's Republic of China, France, Germany, India, Japan, Romania, Russia, Turkey,

Ukraine and the USA, participated in the workshop to review progress made in the field.

SCOPE 57—Particle Flux in the Ocean, edited by V. Ittekkot, P. Schafer, S. Honjo & P.J. Depretis, is published by John Wiley & Sons Ltd, Baffins Lane, Chichester PO19 UD, UK. ISBN 0 471 96073 X, price GBP50.00.

Letter to the Editor

Mervyn Richardson

Dear sir

Re: *IUPAC White Book on Chlorine*

This excellent debate and review of the effects of chlorine, and its compounds, on the environment is very timely (*Pure Appl. Chem.*, 1996, Vol. 68, No. 9). As emphasized by Professor Albert Fischli, President of IUPAC, it is nonsense to consider that such a valuable series of compounds can no longer be used—the benefits to mankind of chlorine-containing substances, such as pharmaceutical, some agrochemicals, colourants, and not least for the disinfection of water is very considerable. It is hoped that this set or articles will receive considerable attention by the popular media and through meaningful debate at scientific and other meetings, and that is noted by politicians.

Perhaps, the paper by Dr Hend Galal-Gorchev of WHO-IPCS deserves special prominence. As she rightfully stresses, the use of chlorine has saved more lives and reduced human suffering from water-borne diseases than any other chemical agent during the past century. This potential has to be increased particularly in the least developed countries as a priority as we enter the 21st century.

One of the greatest potentials of the current decade is the ability for in situ electro-generation of chlorine and its active anions and cations—many of the latter being far more effective in their action against microorganisms than chlorine or hypochlorite alone. Units are now available for in small (and large) communities for the electrogeneration of these active ions which only require an input of electricity which can be generated from a hand generator. vehicle battery/generator, or by solar panels. Hence, even in the World's most difficult terrains, there is no need to be without disinfected water.

Having experienced the problems which result from warfare in Croatia whilst on a mission for the United Nations Industrial Development Organization (UNIDO) in 1993, I would add the use of such units would have been to great advantage. The transport of compressed chlorine gas in war zones on poorly maintained lorries over roads and bridges in an appalling state of repair amounts to the potential of an accident waiting to happen.

Dr. Galal-Gorchev also refers to the use of chlorine alternatives, perhaps ozone being one of the best known. Whilst there is considerable toxicological information relating to the adverse effects of chlorination by-products, the possible toxicological properties of epoxy, oxygen bridge compounds etc. in sub-microgram/liter quantities in water have not received the same attention.

Particular note also needs to be given to the relative ecotoxicology/toxicology and environmental fate of natural compounds to those for xenobiotic substances.

A criticism of this excellent collection of papers relates to the unfortunate omission of attention to risk assessments, risk management, and risk reduction leading to chemical safety. Papers on the economics of the use of chlorine compounds compared with alternatives would have been very welcome, as would have been details on relevant legislation pertaining to emissions of chlorides, chlorine, and chlorine compounds. This is especially so as the legislation for other halogens is not so thorough; think about the considerably higher toxicological effects of bromate.

It is hoped that these papers (The IUPAC White Book) is only the forerunner of a well informed series of scientific reviews which will place the undeniable advantages of chlorine and its compounds in the correct perspective, so that the lay person is aware of the advantages.

Mervyn Richardson,

Principal, Birch Assessment Services for Information on Chemicals (BASIC), 6 Birch Drive, Rickmansworth, Herts, WD3 2UL, UK. Tel./Fax: +44 1923 774187.

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most recent list of the national/regional centres appeared in *Chemistry International* 1995, **17**, 141.

Parameters and symbols for use in nuclear magnetic resonance

NMR is now frequently the technique of choice for the determination of chemical structure in solution. Its uses also span structure in solids and mobility at the molecular level in all phases. The research literature in the subject is vast and ever-increasing. Unfortunately, many articles do not contain sufficient information for experiments to be repeated elsewhere, and there are many variations in the usage of symbols for the same physical quantity. It is the aim of the present recommendations to provide simple check-lists that will enable such problems to be minimised in a way that is consistent with general IUPAC formulation. The area of medical NMR and imaging is not specifically addressed in the recommendations, which are principally aimed at the mainstream use of NMR by chemists (of all sub-disciplines) and by many physicists, biologists, materials scientists and geologists etc. working with NMR.

The document presents recommended notation for use in journal publications involving a significant contribution of nuclear magnetic resonance (NMR) spectroscopy. The recommendations are in two parts: (A) Experimental parameters which should be listed so that the work in question can be repeated elsewhere. (B) A list of symbols (using Roman or Greek characters) to be used for quantities relevant to NMR.

Comments on these recommendations are welcome and should be sent by 31 July 1997 to: Prof. Robin K. Harris, Department of Chemistry, University of Durham, Science Laboratories, South Road, Durham, DH1 3LE. Tel: +44 (191) 3743121; Fax: +44 (191) 3861127; Email: r.k.harris@durham.ac.uk

Definition of terms relating to the non-ultimate mechanical properties of polymers

The document gives definitions of terms related to the non-ultimate mechanical behaviour of polymeric materials, in particular bulk polymers and concentrated solutions and their elastic and viscoelastic properties.

The terms which have been selected are those met in the conventional mechanical characterization of isotropic polymeric materials. They have additionally been limited to those which can be defined precisely and with mathematical rigour. They are arranged in sections dealing with basic definitions of stress and strain, deformations used experimentally, stresses observed experimentally, quantities relating stress and deformation, linear viscoelastic behaviour, and oscillatory deformations and stresses used experimentally for solids.

An index, an alphabetical list of terms and a glossary of symbols are included for ease of reference.

Comments on these recommendations are welcome and should be sent by 31 July 1997 to: Dr. William J. Work, Research Division, Rohm and Haas Co.; PO Box 219, Bristol, Pennsylvania 19007, USA. Tel: +1 (215) 7858549; Fax: +1 (215) 7810624; Email: rbpwjw@rohmhaas.com

Nomenclature of glycolipids

These recommendations update the glycolipid section of The Nomenclature of Lipids (Recommendations 1976), in the light of developments in glycolipid chemistry and biochemistry. The carbohydrate nomenclature used is based on the newly published Nomenclature of Carbohydrates (Recommendations 1996). The recommendations comprise sections on generic terms, principles of nomenclature, classification of glycolipids based on their lipid moieties, neutral glycosphingolipids, acidic glycosphingolipids, and short abbreviations. Semi-systematic names in which trivial names for 'root' structures are used as a prefix are recommended for some neutral glycosphingolipids with oligosaccharide chains. The section on acidic glycosphingolipids addresses gangliosides,

glycuronosphingolipids, sulfoglycosphingolipids, phosphoglycosphingolipids and phosphonoglycosphingolipids.

Comments on these recommendations are welcome and should be sent by 31 July 1997 to: Dr. M. Alan Chester, Blodcentralen, Universitetssjukhuset I Lund, S-221 85, Lund, Sweden. Tel: +46 (46) 173205; Fax: +46 (46) 173226; Email: alan.chester@labmed.lu.se

Nomenclature, symbols, units, and their usage in spectrochemical analysis XIV: Laser-based atomic spectroscopy: Proposal for a new notation

This report is the 14th in a series on Spectrochemical Methods of Analysis issued by IUPAC Commission V.4. Because of the complexity and the lack of uniformity of the present nomenclature (e.g. '2-step excited resonance fluorescence,' 'resonance enhanced multiphoton ionization,' etc.) a new way is needed to describe these transitions. The aim of this document is therefore to present a new notation, the IUPAC notation, to describe the various processes involved in atomic laser spectrochemistry. The notation describes any variety of laser-based atomic spectroscopy as a sequential series of processes which cause transitions between the states of an atom. The processes are symbolized by upper case letters (meanings defined) and modified by lower case subscripts which indicate the state transitions induced by the process, given in a series beginning with the initial state and ending in the final state. The system may be thought of as a means to describe with textual symbols the energy level diagrams often used for this purpose, where the states of an atom are symbolized by a stacked series of horizontal lines and processes are shown as a variety of arrows connecting the states. The notation is not intended to replace or enhance accepted atomic state and transition nomenclature. It is presented rather as a simple system to describe spectrochemical processes. The use of the notation is illustrated with many examples.

Comments on these recommendations are welcome and should be sent by 30 September to: Dr. David S. Moore Managing Editor, Fresenius' J. of Analytical Chemistry Im Maisel 14, D-65232 Taunusstein, Germany Tel: +49-6128-744116 (direct)—7440 (operator); Fax: +49-6128-744420. Email: moore_d@fresenius.com

Copies of the document can be obtained from, and all comments should be addressed to Dr David S. Moore

Conferences

XXX Colloquium Spectroscopicum Internationale, Melbourne, Australia, 21–26 September 1997

IUPAC
SPONSORED

Organised under the auspices of the Royal Australian Chemical Institute Analytical Chemistry Division and the Australian Academy of Science. The XXX CSI is sponsored by IUPAC—International Union of Pure and Applied Chemistry.

Exhibition

XXX CSI 1997 will feature an exhibition of the latest analytical, spectroscopic and associated instrumentation from a wide range of manufacturers. This will be held in the You Yangs Exhibition Hall of the World Congress Centre and conducted over the course of the conference. Exhibits will be arranged in conjunction with the colloquium poster displays giving the highest possible exposure to participants. A meeting room will be made available for company presentations and private discussions. Exhibit areas will be based on multiples of the basic 3 m × 3 m × 2.4 m booths. Those wishing to exhibit products should contact the exhibition co-ordinator;

Dr Trevor Smith, School of Chemistry, The University of Melbourne, Parkville, VIC 3052, Australia. Tel.: +61 3 93446272; Fax: +61 3 93475180.

World Wide Web Homepage updated information may be obtained from the XXX CSI 1997 Homepage on the World Wide Web; http://www.latrobe.edu.au/www/xxxcsi

Registration information

Registration will not be considered complete and submitted abstracts win not be scheduled in the final programme without full payment of fees. Delegates are asked to complete the registration form and forward it, together with payment of fees and accommodation deposit, to the Colloquium Secretariat, before 31 July 1997. The payment must made in Australian Dollars and delegates may pay by either cheque or bankers draft (made payable to XXX CSI in A$). Receipt of registration forms and fees will be acknowledged and accommodation bookings confirmed, shortly after receipt. Please check the confirmation letter and advise the Secretariat of any discrepancies or changes immediately.

Registration will commence at 3:00 pm on Sunday, 21 September, 1997 at the World Congress Centre. The Registration Desk will be attended 8:00 am to 5:00 pm daily throughout the colloquium.

Travel information

Visas

International visitors require a VALID PASSPORT and an ENTRY VISA to enter Australia. It is essential to obtain a visa from your nearest Australian Embassy or Consulate prior to departure as they cannot be obtained upon arrival in Australia. IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting, the IUPAC Secretariat should be notified without delay by the applicant.

IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford, OX4 3YF, UK. Tel.: +44 (0)1865 747744; Fax: +44 (0)1865 747510.

Colloquium Secretariat: The Meeting Planners, 108 Church Street, Hawthorn, Victoria 3122, Australia. Tel: +61 3 98193700; Fax: +61 3 98195978.

Call for papers and posters

Contributed papers for XXX CSI 1997 are now invited. Abstracts are to be sent to;

Dr Simon Lewis, School of Biological & Chemical Sciences, Deakin University, Geelong, Victoria, 3217, Australia. Email: swlewis@deakin.edu.au

The deadline for submission of abstracts is 30 May 1997. Authors will be notified of acceptance or otherwise during June 1997.

Conference calendar

IUPAC sponsored conferences

The following forthcoming conference have been sponsored by IUPAC. Conference circulars and registration forms may be obtained, upon, request, from the names and addresses shown below.

1997

Safety in chemical production

14–15 April

3rd IUPAC Workshop on Safety in Chemical Production: Environmentally Sustainable Manufacture as a Competitive Advantage. San Francisco, CA, USA.

Dr A. M. Ford, Gulf Coast Hazardous Substance Research Center, Lamar University, PO Box 10613, Beaumont, Texas 77710-0613, USA. Tel.: +1 409 880 8768; Fax: +1 409 880 2397.

High temperature materials chemistry

19–23 May
9th International Conference on High Temperature Materials Chemistry (HTMC IX). Pennsylvania State University, PA, USA.
Judy Hall, Conference Planner, Pennsylvania State University, 225 Penn State Conference Center, University Park, PA 16802-7002. Tel.: +1 (814) 8635130. E-mail: conferenceinfo1@cde.psu.edu. WWW site: URL: http://www.cde.psu.edu/C&I/htmc/

Bioorganic chemistry

1–6 June
4th International Symposium on Bioorganic Chemistry. Biarritz, France.
Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45 – 4 Pl. Jussieu, 75252 Paris Cedex 05, France

Molecular architecture for degradable polymers

10–14 June
International Symposium on Molecular Architecture for Degradable Polymers: Molecular Design of Polymeric Materials of Tomorrow. Stockholm, Sweden.
Prof. Ann-Christine Albertsson, Department of Polymer Technology, KTH, Royal Institute of Technology, S-100 44 Stockholm, Sweden. Tel.: +46 (8) 7908274; Fax: +46 (8) 100775.

Electrochemical processes at liquid interfaces and membranes

15–20 June
30th Heyrovsky Conference on Electrochemical Processes at Liquid Interfaces and Membranes, Moravia, Czech Republic.
Prof. Z. Samec, J. Heyrovsky Institute of Physical Chemistry, Dolejskova 3, 182 23 Prague 8, Czech Republic

Polymer synthesis

16–20 June
International Symposium on New Approaches in Polymer Synthesis and Macromolecular Formation. St. Petersburg, Russia.
Mrs Irina Kovalenko (Symposium Coordinator), Institute of Macromolecular Compounds, Bolshoy pr. 31, 199004 St. Petersburg, Russia. Tel.: +7 (812) 2131070; Fax: +7 (812) 2186869; Email: imc@macro.spb.su

Vacuum microbalance techniques

July
27th International Conference on Vacuum Microbalance Techniques. Lublin, Poland.
Dr. P. Staszczuk, Department of Physical Chemistry, Faculty of Chemistry, Marie Curie-Sklodowska University, Pl. Marie Curie-Sklodowsklej 3, 20-031 Lublin, Poland.

Ionic polymerization

7–11 July
International Symposium on Ionic Polymerization. Paris, France.
Prof. F. Cheradame, CNRS, BP 28, 2 rue Henri Dunant, 94320 Thiais, France.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic. Tel.: +42 (2) 360341; Fax: +42 (2) 367891; Email: sympo@imc.cas.cz

Organometallic chemistry

20–25 July
9th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis. Göttingen, Germany.
GDCh, Abteilung Tagungen–OMCOS 9–Postfach 900440, D-60444 Frankfurt A.M., Germany. Fax: +49 (69) 7917475; Email: tg@gdch.de

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules, Surface and Interfacial Phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic. Tel: +42 (2) 360341; Fax: +42 (2) 367891; Email: sympo@imc.cas.cz

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan. Tel.: +81 (3) 38122111 ext. 7261; Fax: +81 (3) 58006945.

Medicinal chemistry

29 July–1 August
AIMECS '97: AFMC International Medicinal Chemistry Symposium. Seoul, Korea.
Prof. Yung Bog Chae, Korea Research Institute of Chemical Technology, PO Box 9, Daedeog-Danji, Daejeon 305-606, Korea.

Pollution

10–13 August 1997
International Conference on Interfaces Against Pollution. Wageningen, the Netherlands.
Conference Secretariat IAP97, PO

Box 8038, NL-6700 EK Wageningen, the Netherlands. Fax: +31 (317) 48377. Email: IAP97@FENK.WAU.NL

Plasma chemistry

18–22 August
13th International Symposium on Plasma Chemistry. Beijing, China.
Dr Lin He, Chinese Society of Theoretical & Applied Mechanics, 15 Zhong Guan Cun Road, Beijing 100080, China.

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
AKM Congress Service, PO Box 37, CH-1218 Le Grand-Saconnex/ GE, Switzerland. Tel.: +41 (22) 7611661; Fax: +41 (22) 7611662.

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion

Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile.
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (2) 6811644; Fax: +56 (2) 6812108; Email: jcostama@lauca.usach.cl

Polymers

25–28 August
12th Bratislava Conference on Polymers: Modified Polyolefins for Advanced Polymeric Materials. Bratislava, Slovak Republic.
12th Bratislava International Conference on Polymers, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, 842 36 Bratislava, Slovak Republic. Tel.: +42 (7) 3782198; Fax: +42 (7) 375923; Email: upolebor@ savba.sk

Solution chemistry

26–31 August
24th International Conference on Solution Chemistry, Centre Omnisport, Vichy, France.
Prof. P. Turq, Laboratoire d'Electrochimie, Université Pierre & Marie Curie, Case courier 51, 4 place Jussieu, 75252 Paris Cedex 05, France.

Electron transfer processes

3–7 September
International Symposium on Electron Transfer Processes and Reactive Intermediates in Macromolecular and Organic Chemistry. Zabre, Poland.
Prof. Z. J. Jedlinski, Institute of Polymer Chemistry, Polish Academy of Sciences, ul. Marie Curie Sklodowskiej 34, 41-800 Zabrze, Poland.

Colloquium spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997. Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel.: +61 (3) 98193700; Fax: +61 (3) 98195978.

Emulsions

23–26 September
2nd World Congress on Emulsions: Industrial Applications of Emulsions. Bordeaux, France.
Mr A. Le Coroller, Directeur-Général, CME, 50 place Marcel Pagnol, 92100 Boulogne-Billancourt, France. Tel.: +33 (1) 47617689. Fax: +33 (1) 47617465.

Macromolecule–metal complexes

6–10 October
7th International Symposium on Macromolecule-Metal Complexes (MMC-7). Noorwijkerhout, Netherlands.
Prof. J. Reedijk, Leiden Institute of Chemistry, PO Box 9502, 2300 RA Leiden, Netherlands. Tel.: +31 (71) 5274459; Fax: +31 (71) 5274451; Email: reedijk@rulgca. leidenuniv.nl

Biodiveristy and bioresources

23–27 November
International Conference on Biodiveristy and Bioresources—Conservation and Utilization. Phuket, Thailand.
Prof. S. Bhumiratana, IUPAC Biodiversity Conference, National Center for Genetic Engineering and Biotechnology, National Science and Technology Development Agency Building, 73/1 Rama VI Road, Bangkok 10400, Thailand. Tel.: +66 (2) 6448150-4, ext. 433, 532, 534; Fax: +66 (2) 6448109.

1998

Trace element speciation

4–7 May
1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences. Neuherberg, Munich, Germany.
First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, FRG. Tel.: +49 (89) 31873030 (2669); Fax: +49 (89) 31873362.

Organic synthesis

30 June–4 July
12th International Conference on Organic Synthesis. Venice, Italy.
Prof. C. Scolastico, Dip.to di Chimica Organica e Industriale, Università di Milano, Via G. Venezian 21, I-20133 Milano, Italy.

Chemistry in Africa

6–10 July
7th International Chemistry Conference in Africa (7th ICCA). Durban, South Africa.
The Secretary, 7th ICC & 34th SACI Convention, Department of Chemistry & Applied Chemistry, University of Natal, Durban 4041, South Africa. Tel.: +27 (31) 3603090; Fax: +27 (31) 2603091; Email: 7icca@che.und.ac.za

Macromolecules

20–23 July
18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.
Dr J. Lukás, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague 6 Petriny, Czech Republic

Chemical thermodynamics

26 July–1 August
15th International Conference on Chemical Thermodynamics. Porto, Portugal.
Prof. M. A. V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal.

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr. John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V OBN. Tel.: +44 (171) 4378656; Fax +44 (171) 7341227.

Solubility phenomena

5–8 August
8th International Symposium on Solubility Phenomena. Niigata, Japan.
Prof. H. Akaiwa, Faculty of Engineering, Gunma University, Kiryu 376, Japan.

Physical organic chemistry

16–21 August
14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.
Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento di Química, 88040-900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy. Tel.: +39 (55) 2757549; Fax: +39 (55) 2757555.

Natural products

October
21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.
Prof. Xiao-Tian Liang, Institute of Materia Medica, Chinese Academy of Medical Sciences, 1 Xian Nong Tan Street, Beijing 100050, China.

2000

Macromolecules

9–14 July
MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.
Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90-363 Lodz, Poland. Tel.: +48 (42) 819815; Fax: +48 (42) 847126.

Biotechnology

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.

Blackwell Science

Osney Mead,
Oxford OX2 0EL,
UK

Telephone
(01865) 206206

Fax
(01865) 206096

INTERNATIONAL JOURNAL OF FOOD SCIENCE AND TECHNOLOGY

Published for the Institute of Food Science and Technology (UK) by Blackwell Science Ltd

Editor: **Dr D G Land**, *Norwich*

The scope of this authoritative journal covers a wide field, ranging from pure research in the various sciences associated with food to practical experiments designed to improve technical processes. While the main object is to provide a forum for papers describing the results of original research, review articles are also included. Manuscripts of original research or comprehensive reviews of specialized sections of food science or technology are welcomed. The editor maintains the high standards of selection and criticism to ensure that only those papers which make a significant contribution to the technology are published. The journal is covered by Current Contents, ASCA and Science Citation Index.

Subscription Information

International Journal of Food Science and Technology is published bimonthly. Subscription rates for 1997 are £235.00 (Europe), £258.00 (Overseas) and US$408.00 (North America).

Order Form

Please tick the appropriate box and return to Karen Edge at the address opposite:

☐ I would like to subscribe to *International Journal of Food Science & Technology*

☐ I wish to pay by cheque and enclose the sum of £_____ US$_____

☐ I wish to pay by Access/American Express/Barclaycard/Diners Card/VISA/Mastercard/JCB (delete as necessary). Please debit my credit card no.

Expiry date_____

with the sum of £____ US$____ Signature_____ Date_____

European Community VAT & Canadian GST

Subscribers in Europe must quote their VAT registration number or state that they are not VAT-registered. Subscribers in the following countries who are not VAT-registered must add VAT to the subscription price at the appropriate rate: Belgium (6% TVA/BTW); France (2.1% TVA); Germany (7% MwSt); Spain (4% IVA); The Netherlands (6% BTW).

All subscribers in Canada must add 7% to allow for GST.

VAT registration number_____ I am not registered for VAT ☐

☐ Please send me a specimen copy of *International Journal of Food Science and Technology*

Name_____

Address_____

_____

Access the Blackwell Science Home Page on http://www.blackwell-science.com

b
Blackwell Science

Osney Mead,
Oxford OX2 0EL,
UK

Telephone
(01865) 206206

Fax
(01865) 206096

Pure and Applied Chemistry

IUPAC

Official Journal of the International Union of Pure and Applied Chemistry

Since 1960 the Union has made available to chemists everywhere a very large amount of important material which it handles each year through its regular publication in Pure and Applied Chemistry. The objectives of the journal are:

- to publish the main invited lectures of symposia sponsored by IUPAC at which authoritative and up-to-date accounts of the subject of the symposium are presented by prominent scientists; the lecturers cover their own recent work and review the worldwide literature on the subject;
- to publish the recommendations of the Union's commissions on nomenclature, symbols and units;
- to publish technical reports on standardization, recommended procedures, collaborative studies, data compilations, etc.;
- to publish critically evaluated state-of-the-art commissioned review articles on important topics.

Subscription Information

Pure and Applied Chemistry is published monthly. Subscription rates for 1997 are for institutions are £672.00 (Europe), £736.00 (overseas) and US$1020.00 (USA & Canada). Individual subscription prices for 1997 are £82.00 (Europe), £82.00 (overseas) and US$115.00 (USA & Canada).

Order Form

Please tick the appropriate box and return to Karen Edge at the address opposite:

☐ Please enter my 1997 Institutional subscription to *Pure and Applied Chemistry*

☐ Please enter my 1997 Individual subscription to *Pure and Applied Chmistry*

☐ I wish to pay by cheque and enclose the sum of £_____ US$_____

☐ I wish to pay by Access/American Express/Diners Card/VISA/Mastercard/JCB

(delete as necessary)

Please debit my credit card no. | | | | | | | | | | | | | | | |

Expiry date _____ with the sum of £_____ US$_____

Signature _____ Date _____

European Community VAT & Canadian GST

Subscribers in Europe must quote their VAT registration number or state that they are not VAT-registered. Subscribers in the following countries who are not VAT-registered must add VAT to the subscription price at the appropriate rate: Belgium (6% TVA/BTW); France (2.1% TVA); Germany (7% MwSt); Spain (4% IVA); The Netherlands (6% BTW).

All subscribers in Canada must add 7% to allow for GST.

☐ Please send me a specimen copy of *Pure and Applied Chemistry*

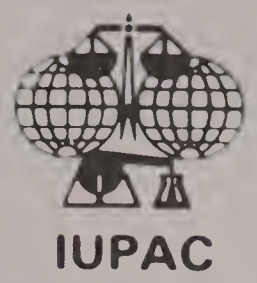
Name _____

Address _____

_____

http://www.blackwell-science.com

International Union of Pure and Applied Chemistry (IUPAC)



President: A. E. FISCHLI (*Switzerland*)
Vice-President: J. JORTNER (*Israel*)
Secretary-General: E. D. BECKER (*USA*)
Treasurer: J. M. WARD (*UK*)

IUPAC Secretariat

Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK.
Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Neue Schweizerisches Chemische Gesellschaft **(Switzerland)**
Türkiye Kimya Dernegi **(Turkey)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1997, Vol. 19, No. 2 (March)

39 Introducing the Working Party on Spectroscopic Data Standards (JCAMP-DX)
Antony N. Davies and Robert Lancashire

41 PAC Review

49 News

52 Recent reports

54 New publications

57 Letter to the Editor
Mervyn Richardson

58 Provisional Recommendations

59 Conference

60 Conference calendar

Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Blackwell Science

0193-6484(199703)19:2:1-9

Printed in Great Britain by Alden, Oxford, Didcot & Northampton

ISSN 0193-6484

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

1997, Vol. 19, No. 3 (May)

Blackwell Science

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

ACTING EDITOR: Mike Ward
PRODUCTION EDITOR: Howard Waller

All correspondence to be addressed to The Editor, Chemistry International, IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK. Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk and http://chemistry.rsc.org/rsc/iupac.htm

Editorial Advisory Board

Chairman:	E. D. BECKER	*Secretary General*		
	E. BUNCEL	*CHEMRAWN Committee*	G. SOMSEN	*Division I*
	A. SMITH	*Committee on Chemistry and Industry*	G. J. LEIGH	*Division II*
	D. H. M. BOWEN	*Committee on Printed and Electronic Publications*	G. SAVELLI	*Division III*
			A. ABE	*Division IV*
	I. M. MILLS	*Interdivisional Committee on Nomenclature and Symbols*	F. INGMAN	*Division V*
			T. R. ROBERTS	*Division VI*
	M. E. PESTANA	*Committee on Teaching of Chemistry*	(To be appointed)	*Division VII*
Acting Secretary:	J.W. JOST	*Executive Director*		

Subscriptions

Six issues of *Chemistry International* will be published bimonthly in 1997. The 1997 subscription rate including postage is GBP 75.00 (UK and overseas except North America) or USD 116.00 (US and Canada). The individual subscription rate is GBP 29.00 (UK and overseas except North America) or USD 42.00 (US and Canada). Microfiche subscriptions are available simultaneously with the printed edition, and microfilm at the end of the subscription year. Subscription orders may be placed directly with IUPAC's official publisher, Blackwell Science Ltd, PO Box 88, Oxford, UK; E-mail: journals.cs@blacksci.co.uk. Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Advertising. Enquiries should be sent to the Advertising Manager, Blackwell Science Ltd, Osney Mead, Oxford OX2 0EL, UK. Telephone: +44 (0) 1865 206206, Telex 83355 Medbok G, Fax +44 (0)1865 721205.

Despatch. The news magazine is despatched within Europe by surface mail, to other continents by various forms of air-speeded delivery: to the US* by air freight for forwarding by periodicals post, to India by air freight for guaranteeed local delivery, and to all other countries by Accelerated Surface Post.

Reproduction of Articles

Unless there is a footnote to the contrary, reproduction or translation of articles in this issue is encouraged, provided that it is accompanied by a reference to the original in *Chemistry International*. The Blackwell Science logo is a trade mark of Blackwell Science Ltd registered at the United Kingdom Trade Marks Registry.
This journal is included in the ADONIS service, whereby copies of individual articles can be printed out from compact discs (CD-ROM) on demand.

*Periodicals postage paid at Rahway, NJ. Post Master, send address changes to *Chemistry International*, c/o Mercury Airfreight International Inc., 2323 Randolph Avenue, Avenel, NJ 07001, USA.

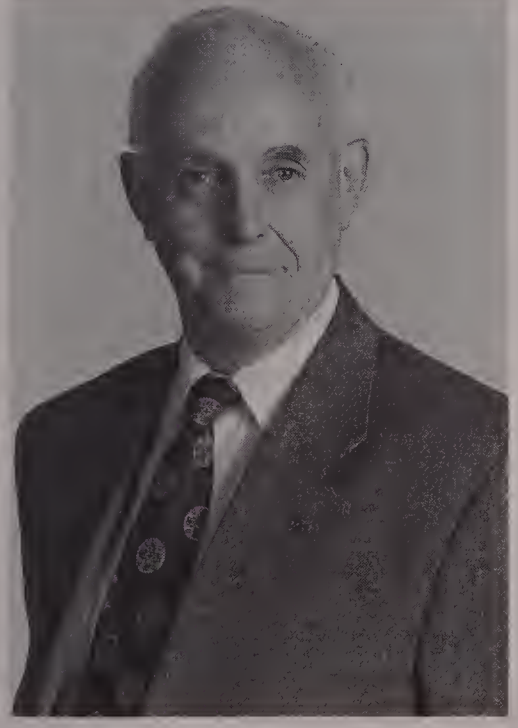
Front cover: Members of the International Council for Chemistry take notes at the inaugural meeting in Paris in January, as Dr Maurizio Iaccorina, UNESCO Assistant Director-General for Science, speaks (see page 67 inside).

International Union of Pure and Applied Chemistry

Retirement of Dr Mo Williams

You may know that Dr Mo Williams retired at the end of April this year after 29 years service as Executive Secretary of the Union. The Officers believe that there are many who have known and been helped by Mo over the years who would like to contribute towards a retirement present, which will be presented to him at the Council Meeting at Geneva in August. I shall be writing separately to past and present Bureau Members, Division Presidents and so on, but I believe that there will be others who would like to contribute. If you are one of those persons, would you kindly send your contribution in US dollars or pounds sterling, if at all possible, to Mrs Erica Sheppard, Assistant Secretary (Finance), IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK. Please make cheques payable to IUPAC (MW).

J. M. Ward
Treasurer



Dr Mo Williams

...appointment of new Executive Director

John W. Jost is the new Executive Director of IUPAC, replacing Dr Mo Williams. Jost will organize and direct the IUPAC Secretariat when it moves to Research Triangle Park, North Carolina, USA, later this year (see page 94).

Jost comes to the IUPAC post from international oil company Unocal, where he has held managerial and executive positions. Born in Germany, Jost moved as a child to the USA, where his education and career have been centred. He received Bachelor's and Master's degrees in chemistry from Columbia University, obtained his PhD in physical chemistry from the State University of New York in Stony Brook in 1971, and did post-doctoral research at the University of California in Berkeley. He had been at Unocal since 1974, serving in recent years as Senior Vice-President for Administration, President of Unocal Process Technology and Licensing, and Vice-President of the Fred L. Hartley Research Center.

IUPAC President Albert Fischli points out that Jost's appointment comes against a backdrop of intensive evaluation of IUPAC's mission and plans for restructuring of the organization, which was founded in 1919. Fischli adds: 'Dr Jost has superb qualifications to organize and manage the new Secretariat. I expect that he will build on the successes of our Secretariat under Mo Williams and will introduce enhancements to permit the Union to meet the challenges of the coming years'.

To ensure continuity, transfer of functions to Research Triangle Park from the present Secretariat in Oxford will be gradual. The administrative staff in Oxford will remain intact until after the biennial IUPAC General Assembly, to be held in Geneva, Switzerland, 23–30 August.

Dr John Jost

Meeting on future directions for IUPAC

Eight leaders in chemistry and the chemical industry from eastern and western Europe met with the IUPAC Officers at the Royal Society, London, UK, on 24 February 1997, to discuss future roles for IUPAC. This meeting was a follow-up to a similar 'brainstorming' session held in North America last June. Building on the recommendations of that meeting, the group in London was asked to address a number of points, including:

a Reconsideration of the objectives of the Union
b Priority areas of the Union
c The balance between basic academic research and industrial R&D
d The service of chemistry to society and to the international community
e Global important issues in chemistry
f Contribution to developing countries
g The role of the Union in chemical education at all levels
h International communication in the chemistry community
i The organization of IUPAC

The full report of this meeting, to be presented formally to the Bureau at its next meeting, includes 21 recommendations. Some highlights are as follows:

- IUPAC's objectives, as given in its Statutes, refer largely to *means* rather than *ends*. IUPAC should develop specific *goals* which can be expressed succinctly in compelling terms that are attractive and easily understood by chemists and the chemical industry.
- The strength of IUPAC is in its global position. It should undertake projects of true international dimensions.
- IUPAC should provide information in understandable form to governments and the public in order to make clear the role of chemistry and chemicals in the world. IUPAC should limit its presentations to facts and avoid political judgements.
- IUPAC should make greater efforts to improve its image by explaining to chemists and the chemical industry just how the large underlying structure contributes to the progress of chemistry.
- Better dissemination of information by IUPAC is needed at all levels. Distribution of IUPAC Recommendations via the Internet (which is doubling in size every two months) would bring this information to many chemists who often find the printed nomenclature books inaccessible.
- IUPAC should reach out to embrace chemical aspects of interdisciplinary fields which have a significant chemistry component, for example molecular biology, biotechnology and materials science. IUPAC should hold conferences to demonstrate the central role of chemistry in many interdisciplinary fields.

Edwin D. Becker,
Secretary General, IUPAC

- IUPAC should place more emphasis on projects that are focused on achievable goals and are completed as quickly as possible. Assistance from an adequate professional staff is needed to help overcome the perception that IUPAC's work is slow and inefficient. IUPAC should consider how to form a 'think tank' or advisory apparatus to develop broad-based projects that might not be initiated through the current organizational structure.
- IUPAC should address a number of organizational issues, including a careful examination of whether the current Divisional structure along traditional chemical disciplines is still optimum and whether Commissions are too large and/or too numerous. More interdisciplinary programmes are needed.
- The traditional role in chemical nomenclature remains important, but implementation via the various Nomenclature Commissions should be re-examined in detail.

The eight chemistry/chemical industry leaders present were: David Culpin, Director, UK Chemical Industries Association; Prof. Dr Heindirk tom Dieck, Executive Director, Gesellschaft Deutscher Chemiker; Prof. Oleg M. Nefedov, Chairman, National Committee of Russian Chemists, Russian Academy of Sciences; Prof. Guy Ourisson, Vice-President, French Academy of Sciences; Prof. Lord George Porter, Department of Biology, Imperial College, London; Dr H. Luzius Senti, Corporate Vice-President, Firmenich SA, Geneva; Prof. Dr Andrea Vasella, Laboratorium für Organische Chemie, ETH Zentrum, Zürich; Prof. Rudolph Zahradnik, President, Czech Academy of Sciences. The IUPAC Officers present were: Prof. Albert E. Fischli, President; Prof. Joshua Jortner, Vice-President; Dr Edwin D. Becker, Secretary General; Prof. John M. Ward, Treasurer; Dr John M. Jost, Executive Director Designate.

Edwin D. Becker

IUPAC and UNESCO inaugurate International Council for Chemistry

The International Council for Chemistry (ICC), a high level advisory body to IUPAC and UNESCO (the United Nations Educational, Scientific and Cultural Organization), held its inaugural meeting in Paris, France, on 31 January 1997. The ICC is to provide guidance in the development of programmes to promote international cooperation in the chemical sciences, allied interdisciplinary areas and chemistry education. It will assist in identifying partnerships in research and training and in facilitating dialogue among the scientific community, governments, industry and society at large.

The ICC is chaired by IUPAC President Albert Fischli. Prof. Vladimir Zharov, Director of the Basic Sciences Division of UNESCO, is Executive Secretary.

The opening session of the ICC meeting was addressed by Dr Maurizio Iaccorina, UNESCO Assistant Director-General for Science, who urged the Council to 'think big' in terms of activities that will be of benefit to the developing world and can generate appropriate governmental support. Dr Iaccorina pointed out that UNESCO, like IUPAC, is not a 'funding agency' for large projects but rather attempts to provide initial support for innovative projects and to seek extra budgetary support where appropriate.

President Fischli's opening remarks stressed the importance of chemistry as a central science, which has a major impact on health, the environment, development of materials and other areas of technology. He described IUPAC's overall structure and its worldwide membership of 39 National Adhering Organizations, 16 Observer Countries, 30 Associated Organizations, 160 Company Associates and more than 5000 Affiliate Members, and he summarized the role of IUPAC-sponsored conferences, publications and other activities in contributing to the international development of chemistry.

Spirited discussion characterized the meeting, as all members of the Council entered into dialogue on matters ranging from the fundamental question of whether such a Council is needed in view of other existing organizations, to specific ideas for potentially valuable projects. The group concluded that such a Council could perform a useful service in increasing the awareness of the public at large, decision makers, governments and donor agencies to the opportunities offered by chemistry. They decided that the ICC will aid the development of UNESCO-IUPAC programmes with focus on:

- the advancement of pure and applied chemistry and its full use for the development of society;
- the promotion of North-South cooperation in advanced training and research in the chemical sciences as well as in chemistry education;
- the development and coordination of partnerships between specialized international and regional organizations dealing with topics of a chemical nature;
- the transfer to less developed countries of information in the chemical sciences and assistance for building their national technical capabilities;
- the promotion of cooperation between science and industry;
- chemistry for UNESCO's Agenda 21 and environmentally sustainable development;
- fund-raising for major international and regional projects in chemistry through partnership with UNESCO, UNIDO, WHO, OECD, ICSU, international and national foundations, academies of science, chemical societies, networks and industrial science-based enterprises.

The ICC membership is drawn from world leaders in chemistry and science policy, and includes four Nobel Laureates. In addition to Profs Fischli and Zharov, membership includes Dr Chris F. Garbers (South Africa), Prof. Dudley R. Herschbach (USA), Dr Yoshikazu Ito (Japan), Prof. Jean-Marie Lehn (France), Prof. Alejandro C. Paladini (Argentina), Prof. John C. Polanyi (Canada), Prof. Lord George Porter (UK) and Prof. C.N.R. Rao (India). An Executive Committee, consisting of Profs. Fischli and Zharov, along with IUPAC Officials Dr Edwin D. Becker (Secretary General), Dr Rene-Paul Martin (Chairman, COCI) and Dr Alan Hayes (Chairman, CHEMRAWN Committee), will take steps to implement policy set by the Council.

Edwin D. Becker

Dr Maurizio Iaccorina, UNESCO Assistant Director-General for Science (left), presents opening remarks at the inaugural meeting of the International Council for Chemistry.

IOCG Crystal Growth Awards: call for nominations

The International Organization for Crystal Growth (IOCG) sponsors two triennial prizes: the IOCG Frank Prize, presented for significant contributions in fundamental aspects of crystal growth, and the IOCG Laudise Prize, presented for significant contributions in the technological aspects of crystal growth. Both awards are made for outstanding contributions through technical achievements, publications and presentations, and their impact world-wide on science and technology. The awards consist of a commemorative item plus an invitation to present the work at the relevant ICCG.

The awards were first made at ICCG-9, to A.A. Chernov (Frank Prize) and J. Nishizawa (Laudise Prize). At ICCG-10 the recipients were R.F. Sekerka (Frank Prize) and V.V. Osiko and J.F. Wenckus (joint Laudise Prize). At ICCG-11 the awards were made to Bennema (Frank Prize) and Feigelson (Laudise Prize).

The next awards will be presented during ICCG-12 in Jerusalem, Israel, on 26–31 July 1998. Nominations for these awards, together with supporting documentation (six copies), should be sent before 15 September 1997 to the IOCG Awards Chairman, Prof. T. Nishinaga, at the address below, for consideration by the IOCG Awards Committee.

Nominations should include the candidate's title, position, age, postal address, curriculum vitae, list of publications and a citation which describes his/her work and its relevance to the field of crystal growth. It should be made clear for which prize the submission is being made. Nominations can be made by national associations for crystal growth or by individuals, but not by candidates themselves. Nominators should append their own name, title, address, E-mail and position, as well as their signature.

Nominations for the 1998 prizes should be sent to:

Prof. T. Nishinaga, President of IOCG, Department of Electronic Engineering, The Graduate School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan, Tel.: +81 3 3812 2111 ext 6673, Fax: +81 3 5684 3974 or +81 3 3818 5706, E-mail: tatau@ee.t.u-tokyo.ac.jp

IUPAC proposes names for transfermium elements

The Commission on Nomenclature of Inorganic Chemistry (CNIC) has presented a revised list of recommended names for elements 101–109. The revision is based partly on suggestions received during the official five-month comment period called for by IUPAC's by-laws. Comments came from individual chemists world-wide and from the 39 National Adhering Organizations (NAOs) that comprise IUPAC. The new names replace the provisional recommendations initially proposed by CNIC in August 1994. Major changes include the recommendation of seaborgium for element 106; hassium, rather than hahnium, for 108; the retention of rutherfordium for 104; and the adoption of dubnium for 105.

The naming of the transfermium elements has been controversial, partly because of disagreements on priority for discovery of several elements. According to Alan Sargeson, Chairman of CNIC, the Commission accepted the conclusions on discovery reached by the Transfermium Working Group (TWG) in 1993. The TWG was formed jointly by IUPAC and the International Union of Pure and Applied Physics in 1986 to establish criteria that must be satisfied for the discovery of a new chemical element to be recognized and to evaluate competing claims. In selecting names, CNIC gave great weight to proposals by discoverers of the elements but considered other factors as well. The current recommendations were developed by CNIC after dropping its previous restriction of not naming an element for a living person. According to Sargeson: 'The response from NAOs and the chemical community showed quite clearly that chemists in general did not see this as an important issue and many thought it was irrelevant. The Commission therefore did not appear to reflect general chemical opinion on this issue'.

IUPAC President Albert Fischli complimented CNIC and the President of the Inorganic Chemistry Division of IUPAC, Jeff Leigh, on their conscientious efforts to forge a consensus on a difficult issue. 'IUPAC's responsibility is to develop recommendations that are widely accepted and that can form the basis for international communication in chemistry', said Fischli. 'Our standard process of proposing provisional recommendations, soliciting comments from the chemistry community and making revisions where indicated has

Prof. Glenn T. Seaborg

worked well. Unfortunately, with conflicting claims and preferences, it has not been possible to devise names that are completely satisfying to all the laboratories involved in these discoveries. I believe that the proposal from CNIC comes close to achieving our goal. Nevertheless, these names will not have final IUPAC endorsement until they are approved by our Council, which meets in Geneva in August. The delegations from our 40 member countries will have the final say'.

The names and symbols recommended by CNIC are as follows:

Element	Name	Symbol
101	Mendelevium	Md
102	Nobelium	No
103	Lawrencium	Lr
104	Rutherfordium	Rf
105	Dubnium	Db
106	Seaborgium	Sg
107	Bohrium	Bh
108	Hassium	Hs
109	Meitnerium	Mt

The Commission recommended that elements 101, mendelevium; 102, nobelium; and 103, lawrencium, should retain their commonly accepted names although it is clear that the original claim of discovery of nobelium is in error. The priorities for the discovery of elements 104 and 105 are disputed. CNIC accepted the name proposed for 104 by the Berkeley group, rutherfordium, and recommended that element 105 should be called dubnium in honour of the Dubna laboratory, where important contributions to the creation of transfermium elements have originated. It should be noted that the contributions of the Berkeley laboratory have been recognized several times in this same way. Element 106 was uncontested as a discovery, and the name seaborgium (Sg) was accepted. Elements 107, 108 and 109 are also uncontested discoveries and CNIC accepted the proposals of the discoverers in the Darmstadt group, except for bohrium, rather than nielsbohrium for 107, after consultation with Danish authorities.

Names and Addresses

Full details (names, addresses, telephone/telex/fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* 1995, **17**(6), 215–226. The IUPAC Secretariat has been notified of the following changes:

Prof. Ann-Christine Albertsson (Chairman, Commission IV.3). E-mail: aila@polymer.kth.se

Prof. Manfred Grasserbauer (President, Analytical Chemistry Division), Institute for Reference Materials and Measurements, European Commission - JRC/IRMM, Retieseweg, B-2440 Geel, Belgium. Tel.: +32 14 571 292/293 (Sec); Fax: +32 14 584 273; E-mail: manfred.grasserbauer@jrc.org

Dr Anders Kallner (President, Clinical Chemistry Section). E-mail: Kallner_Anders/cc@cc.ks.se

Prof. Michael W. Linscheid (Secretary, Commission V.2).

Dr René-Paul Martin (Chairman, COCI), Elf Atochem, DRH, 4 cours Michelet, F-92071 Paris La Defense Cedex, France.

Dr J. R. Moody (Chairman, Commission II.4). Fax: +1 301 977 8392; E-mail: john.moody@nist.gov

Dr David S. Moore (Secretary, Commission V.4), Fresenius Journal of Analytical Chemistry, Im Maisel 14, D-65232 Taunusstein, FRG.

Dr Willie J. G. M. Peijnenburg (Secretary, Commission VI.3). E-mail: WJGM.Peijnenburg@rivm.nl

Dr Kenneth D. Racke (Chairman VI.4), Dow Elanco, 9330 Zionsville Road, Building 308/2E, Indianapolis, Indiana 46268-1053, USA. Tel.: +1 317 337 4654; Fax: +1 317 337 4649; E-mail: kracke@dowelanco.com

Prof. Roger M. Smith (Secretary V.3). E-mail: R.M.Smith@lboro.ac.uk

Dr Pieter G. Thiel (Chairman, Commission VI.5). Tel.: +27 21 9380911

Prof. William Wakeham (Chairman, Commission I.2), Sherfield Building, Imperial College of Science, Technology and Medicine, Prince Consort Road, London SW7 2AZ. Tel.: +44 171 594 5005; Fax: +44 171 594 8802; E-mail: w.wakeham@ic.ac.uk

IUPAC colleague deceased

China: Prof. Lu Xiankun (28 November 1996), Chinese Chemical Society, Commission on Fundamental Environmental Chemistry (1992–).

Commission News

Summary Minutes from the Meeting of the Commission on High Temperature Materials and Solid State Chemistry (II.3), Grenoble, France, 14–16 June 1996

Following the 1995 meeting in Guildford, Commission II.3 has continued to work partly in classical IUPAC nomenclature and standardization areas while also pursuing projects related to chemistry in the service of mankind, particularly projects addressing topical areas in inorganic materials.

At Guildford and subsequently the Commission listened to, considered and formulated plans to act on major concerns of the Union. New members were carefully chosen to provide additional substantial expertise in solid state materials. The 1996 Grenoble meeting was the first participated in by these new members.

Following publication of *Recommended Terminology for the Description of Carbon as a Solid* in 1995, a monumental achievement from some 20 years of dedicated work by Prof. E. Fitzer and about 50 scientists, the Commission under Prof. H.-P. Boehm started a new subcommittee to address standardization of characterization methods of carbon materials. National standards differ in important parameters. Many of the national standards for the characterization of carbon materials compiled in a 1979 Commission II.3 IUPAC publication are outdated. The objective of the current project is to collect the relevant up-to-date standards from various national standard organizations, to point out differences, and to seek for each method an expert's comments on the effect of such differences. By contacting the various national groups and holding meetings at the annual international Carbon conferences the subcommittee is obtaining participation by the most prominent scientists in the area.

The Commission is working on several terminology projects addressing problems of worldwide importance in the industrial manufacture of specialized inorganic materials: *Terminology used in Sol-Gel Processing of Advanced Ceramics and Inorganic/Organic Polymeric Substances* (a pool project with Commission IV.1), *Terminology of Vapor Deposition Techniques, Terminology of Silicon Nitride based Ceramic and Related Materials* and *Terminology for Diffusion in the Solid State*.

Results from two Commission projects have been published in *Pure and Applied Chemistry*: *Quantitative Analysis of a PbO-SiO_2 Glass by Electron Microprobe* and *The Electrical Conductivity of Cubic Stabilized Zirconia*. These publications report the results and analysis of comparative experimental work performed in different laboratories on identical samples and offer important conclusions regarding the reliability and limitations of measurements in these areas.

The Commission also approved for publication a manuscript on the *Characterization of SiC Powders*.

Utilizing the Commission's expertise in inorganic materials, in particular its expertise with materials prepared or used at high temperatures, are two projects devoted to ceramic materials: *Chemical Research Needed to Improve High Temperature Processing of Ceramics* and *Surface Analysis of Ceramics*. The Commission received and considered detailed reports on the material to be included in those publications at Grenoble.

Another important area of Commission activity is to promote education in the fields of solid state and high temperature chemistry. After compiling *A Selection of Textbooks and Reference Literature in English on Solid State Chemistry and Related Areas*, a companion project is in progress to gather a set of checked and tested experiments illustrating important aspects of solid state chemistry. The Commission is also looking into a potential project on *Teaching of High Temperature Chemistry at University.*

The Commission continues its highly successful series of conferences on high temperature materials chemistry. HTMC IX is being held at Penn State University this month; Juelich, Germany, has been chosen as the venue for the 10th IUPAC HTMC conference to be held in 2000. HTMC-X will be organized by Prof. Hilpert.

The next meeting will be held in Geneva, Switzerland, on 24–26 August 1997.

Prof. Dr Drago Kolar
(Secretary of Commission II.3)

Summary Minutes from the Meeting of the Commission on Physical Organic Chemistry (III.2), Inchon, Korea, 30–31 August 1996

Two major results were recorded during the 1996 series of meetings of the Commission in Inchon. The first result concerns the practical completion, in less than one year, of the project *Physical Organic Chemistry for*

Commission of Physical Organic Chemistry. Standing, from left to right: Z. Rappoport, J.-L.M. Abboud, P. Müller, J. Shorter, E. Baciocchi, E. Humeres, G.-Z. Ji, C.L. Perrin, D. Lenoir, Y. Takeuchi. Sitting from left to right: M.-F. Ruasse, T.T. Tidwell, T.A. Modro, P. Tundo.

the 21st Century. A total of 20 essays written by distinguished scientists in different areas, including the Nobel Prize recipient George A. Olah, have been collected and this material, with a Foreword by Prof. C.L. Perrin and a Prologue by Prof. T.T. Tidwell, has been published in the February 1997 issue of *Pure and Applied Chemistry* (see page 74). The Commission is certain that this document will provide the chemical community and particularly the practitioners and the students of physical organic chemistry with a survey of expert opinions about the future of this discipline, the most promising directions, the opportunities and the challenges.

The second result is the Commission approval for the initiation of two projects in the area of Environmental Chemistry. One project should deal with the *Evaluation of Physical and Chemical Properties of Environmentally Important Organic Compounds;* the other, with the *Pathways of Environmentally Benign Organic Chemistry*. It is hoped that both projects will be submitted to the Division of Organic Chemistry during the 39th IUPAC General Assembly in Geneva.

The Commission was also very pleased to note that the project *Compilation and Critical Evaluation of Structure-Reactivity Parameters. Part II* has been completed and is on the way to be published. Appreciation was also expressed for the projects *Glossary of Terms Used in Theoretical Organic Chemistry* and *Critical Compilation of Scales of Medium Effects,* both in their final stage. Substantial progress was reported for the other ongoing projects, namely *Guidelines for the Publication of Research Results from Empirical Force Field Calculations* and *Glossary of Terms Used in Supramolecular Chemistry*.

In addition to those related to the environmental chemistry, other possible future projects were discussed by the Commission. Particular attention was paid to projects on *Materials, Chemical Education* and *Gas-Phase and Solution Data of Carbocations*. For the latter, an initiation proposal will be presented by Prof. J.-L.M. Abboud in the 1997 meeting in Geneva.

The Commission has expressed full appreciation for the organization of the 13th IUPAC Conference on Physical Organic Chemistry (ICPOC) as well as for the quality of the scientific programme.

Fully aware of the importance of the dissemination of its results, the Commission has immediately taken advantage of the fact that IUPAC is now on the Internet. Thus, the *Glossary on Physical Organic Chemistry* is already present on the IUPAC Home Page. Other documents will soon follow. Thanks to Dr Zdysiewicz, some documents of the Commission have also been put on the Home Page of the *Australian Journal of Chemistry*.

The Commission also discussed some topics concerning the activities of the Union and in this context firm opposition was expressed to the proposal by the IUPAC President of merging the Divisions of Organic and Inorganic Chemistry.

Finally, it was decided to propose that the 15th ICPOC in 2000 will be held in Göteborg (Sweden). The next series of meetings of the Commission will take place in Geneva on 24–26 August 1997.

Prof. T.T. Tidwell (Chair) and Prof. E. Baciocchi (Secretary)

PAC review

***Pure and Applied Chemistry* (PAC) is the official journal of IUPAC. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in PAC are published in *Chemistry International* in the section Recent Reports. In this section we take a brief look at symposia and lectures published in recent issues of PAC.**

Lectures from Conference

The March 1997 issue of *Pure and Applied Chemistry*, **69**(3), contains texts of the plenary, mini-symposium and invited lectures presented at the 11th International Conference on Organic Synthesis, held in Amsterdam, the Netherlands, 30 June–4 July 1996. The conference was organized by the Organic Chemistry Division in conjunction with the Royal Netherlands Chemical Society.

Among the seven plenary lectures was one on rearrangement strategies in natural products synthesis, presented by Andrew S. Kende of the Department of Chemistry, University of Rochester, Rochester, New York, in which he described an unexpected molecular rearrangement first encountered during a recent alkaloid synthesis. He also reported the exploitation of the pH-dependent equilibrium between hydroxy-lactams and the isomeric amino-lactones as a key strategic element in some recent total syntheses from the Rochester laboratories.

Over the last decade Kende's group has targeted several natural product syntheses in which amide rearrangements are a central element of strategic design. Such targets include the macrolide antibiotic Lankacidin C, the antitumour agent didesepoxyrhizoxin and the rare acaricidal and antitumour alkaloid altemicidin. In particular, he reported the first total synthesis of (-)-altemicidin by an enantioselective route employing a lactone to lactam amide rearrangement, in which a bicycloheptane-derived lactone is converted quanititatively to an azaindane system.

The other six plenary lectures at the conference covered: recent advances in the synthesis of anti-fungal agents; synthetic heparin-like antithrombotics; covalent fullerene chemistry; enzyme inhibitors, synthesis and approach to mechanism; total synthesis of selected natural products; and a chemo-enzymatic approach to the study of carbohydrate-based biological recognitions.

The mini-symposium addressed syntheses directed towards complex medicinal agents. Included was a presentation from Ichiro Shinkai of the Merck Research Laboratories in New Jersey on the significant impact of recent progress in asymmetric syntheses on strategies for drug development in the pharmaceutical industry. Under recent guidelines by the US Food and Drug Administration, many drug firms are no longer considering the development of racemic forms of chiral drugs, he explained. Shinkai drew on examples of stereoselective syntheses of drug candidates discovered and developed by Merck, including the leukotriene antagonists for the treatment of asthma; MK-499, a potent potassium channel blocker under investigation for the treatment of ventricular arrhythmias and the prevention of sudden cardiac death; HIV protease inhibitor MK-0639; and reverse transcriptase inhibitors L-738,372 and L-743,726.

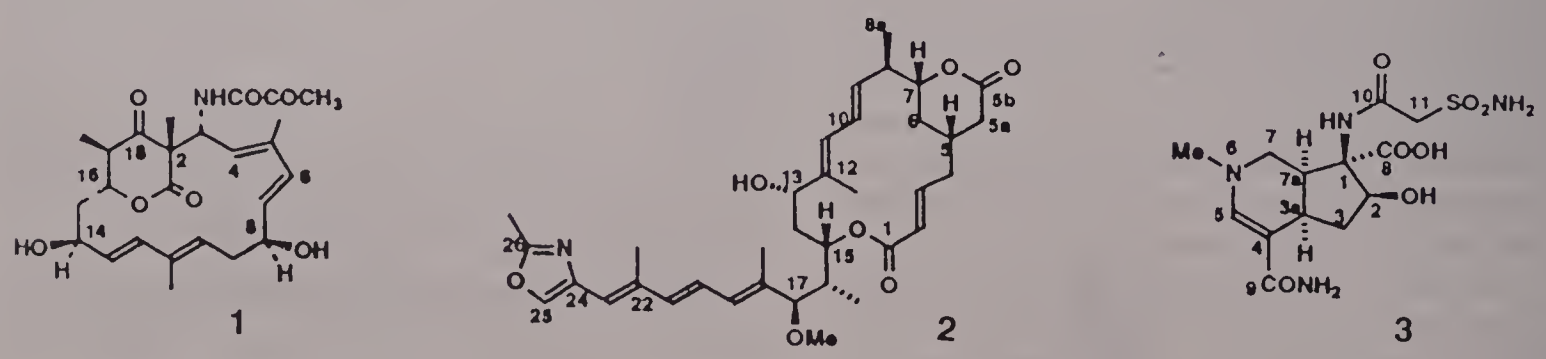


Fig. 1 Targets of natural product synthesis: (1) Lankacidin C, (2) didesepoxyrhizoxin, (3) altemicidin.

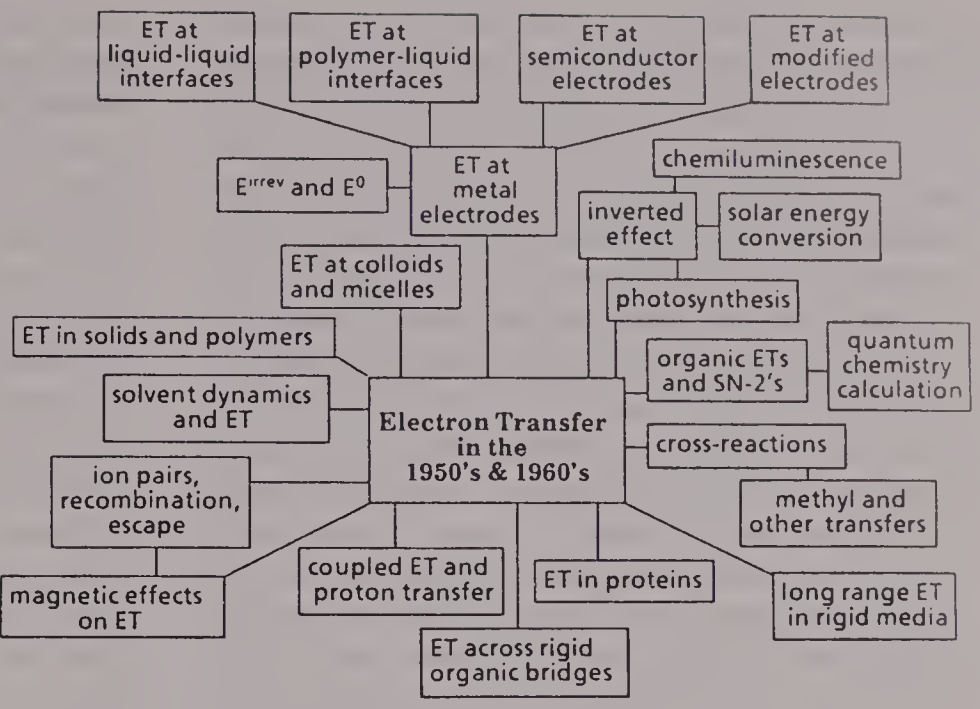


Fig. 2 Examples of topics in the electron transfer field.

The other presentations at the mini-symposium were: towards chemical libraries of annonaceous acetogenins; plant cell culture combined with chemistry—routes to clinically important compounds; backbone modifications for antisense oligonucleotides; discovery of endothelin antagonists; developing a general strategy for the solid supported synthesis of heterocycles—applications to the generation of molecular diversity and drug discovery; synthesis of oligosaccharide mimetics; tetrathiafulvalenes in macrocyclic and supramolecular chemistry.

Lectures from Congress

The January 1997 issue of *Pure and Applied Chemistry*, **69** (1), contains the texts of the plenary and selected invited lectures presented at the 35th IUPAC Congress held in Istanbul, Turkey, 14–19 August 1995. The Congress, held in conjunction with the Turkish Chemical Society, covered a diverse range of subjects. The three plenary lectures were given by: Jack G. Calvert, Senior Research Associate at The National Center for Atmospheric Research, Boulder, Colorado, on the chemistry of the atmosphere and its perturbations through human activities; R.A. Marcus of the Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California, on electron transfer reactions in chemistry; and Pavel Nikolaev, Andreas Thess, Ting Guo, Daniel T. Colbert and Richard E. Smalley of the Center for Nanoscale Science and Technology, Rice Quantum Institute and Departments of Chemistry and Physics, at Rice University, Houston, Texas, on fullerene nanowires. Some 27 invited lectures are also included in the PAC volume.

In his plenary lecture, Jack Calvert reviewed the chemistry of the atmosphere, the major environmental challenges in atmospheric chemistry—stratospheric ozone depletion by aircraft emissions, tropospheric ozone build-up, global warming, acid deposition etc., and current and future participation of IUPAC scientists in the solution of atmospheric and environmental chemistry problems. In particular, he concluded that, as the economies of the rapidly developing countries grow and as new technologies appear in all societies, the identification of perturbations induced in the chemistry of the atmosphere, and in the environment in general, will become increasingly important. Furthermore the understanding of the fundamental chemistry of the effects induced will be a crucial part of the development of scientifically sound emissions control strategies for the impurities which lead to these perturbations. In the process of development of sound environmental policies, Calvert suggested that a high priority be placed on the involvement of interested IUPAC scientists in the many chemical disciplines. IUPAC's unique international mix of chemists from a large variety of workplaces, academic, industrial, government and private sectors offers a pool of expertise which is uniquely qualified to apply fundamental principles to the solutions of environmental problems and to train scientists in the developing countries in the basic and applied areas of environmental chemistry.

R.A. Marcus presented an insight into the history and recent trends and described his own involvement in the field of electron transfer processes, a field that has grown enormously, both in chemistry and biology, since the late 1940s. In outlining the history, Marcus explained that the early experiments in the electron transfer field were on 'isotopic exchange reactions' (self-exchange reactions) and later 'cross reactions'. These experiments reflected two principal influences. One of these was the availability after the Second World War of many radioactive isotopes, which permitted the study of a large number of isotopic exchange electron transfer reactions in aqueous solution. There is a two-fold simplicity in typical self-exchange electron transfer

reactions (so-called since other methods beside isotopic exchange were later used to study some of them): the reaction products are identical with the reactants, thus eliminating one factor which usually influences the rate of a chemical reaction in a major way, namely the relative thermodynamic stability of the reactants and products; and no chemical bonds are broken or formed in *simple* electron transfer reactions. Indeed, these self-exchange reactions represent, for these combined reasons, the simplest class of reactions in chemistry. Observations stemming directly from this simplicity were to have major consequences, not only for the electron transfer field but also, to a lesser extent, for the study of other kinds of chemical reactions as well.

A second factor in the growth of the electron transfer field was the introduction of new instrumentation, which permitted the study of the rates of rapid chemical reactions. Marcus cited the example of the stopped-flow apparatus, pioneered for inorganic electron transfer reactions by N. Sutin. It permitted the study of bimolecular reactions in solution in the millisecond time scale (a fast time scale at that time). Such studies led to the investigation of what has been termed electron transfer 'cross reactions', i.e. electron transfer reactions between two different redox systems, which supplemented the earlier studies of the self-exchange electron transfer reactions. A comparative study of these two types of reaction, self-exchange and cross reactions, stimulated by theory, was also later to have major consequences for the field and indeed for other areas.

Again, in the field of electrochemistry, the new post-war instrumentation in chemical laboratories led to methods which permitted the study of fast electron transfer reactions at metal electrodes. Prior to the late 1940s only relatively slow electrochemical reactions, such as the discharge of an H_3O^+ ion at an electrode, to form H_2 had been investigated extensively.

Returning to the present, Marcus pointed out that numerous electron transfer studies have now been made in other areas, many made possible by a newer technology, lasers particularly, and now include studies in the picosecond and subpicosecond time regimes. Just recently, (non-laser) nanometre-sized electrodes have been introduced to study electrochemical processes that are still faster than those hitherto investigated. Still other recent investigations, important for testing aspects of the electron transfer theory at electrodes, involve the new use of an intervening ordered adsorbed monolayer of long chain organic compounds on the electrode to facilitate the study of various effects, such as varying the metal-solution potential difference on the electrochemical electron transfer rate.

In their plenary lecture, Pavel Nikolaev *et al.* reported their work on 'fullerene nanowires'—hollow carbon tubes 1.2–1.4 nm in diameter, more than 20 μm in length, constructed of a single hexagonally bonded graphene sheet wrapped into a cylinder, with hemispherical endcaps involving six pentagons. The work is aimed at producing a 'dream' fibre—expected, for example, to exhibit a tensile strength roughly 100 times higher than that of steel, while having less than one-fifth the weight. In the form of a multistrand rope (10^{14} strands/cm^2) this fibre would provide the ultimate structural cable. Its thermal conductivity along the fibre axis should be extremely high—similar to that of diamond. But most intriguing, say the scientists, would be the electrical properties. It would be metallic. Particularly when doped with metal atoms arrayed like peas in a pod down the central axis, or 'intercalated' in the spaces between adjacent tubes in a multistranded composite, the electrical conductivity of these nanoscale wires at room temperature may be dramatically higher than gold. They imagine these fullerene wires replacing power cables, or used individually to interconnect electronic devices on a molecular scale.

In reality, Nikolaev *et al.* acknowledge that it would be necessary to 'trick' carbon into assembling in this way—there is no question that these hollow cylinders are not the most stable possible form of carbon. However, they believe they may have found just such a trick. They report producing nanowires in high yield by laser vaporization of a composite rod of graphite with 1–2 atom percent of a catalyst such as 1/1 Ni/Co, inside a quartz tube at 1200 °C, in a 1 cm/s flow of argon at 500 Torr. The yield is greater than 50% of all the carbon vaporized. the wires are found to be aligned to form ropes of 10–100 parallel tubes held together in a closed-packed hexagonal array by van der Waals forces. The ropes are often found with overall length greater than 0.1 mm. Due to their expected high electrical conductivity, especially when doped with metals either down the hollow inside region or on the outside, intercalated in the triangular gaps between the adjacent tubes, these new materials may provide the first source of wires on the nanometre scale whose electrical conduction is truly metallic.

A Symposium in Print

The February 1997 issue of *Pure and Applied Chemistry*, **69** (2), contains plenary lectures which comprise *Physical Organic Chemistry for the 21st Century: A Symposium in Print,* organized by IUPAC Commission III.2 on Physical Organic Chemistry. In a foreword, C.L. Perrin of the University of California, San Diego, explains the reasoning behind the symposium. Historically physical organic chemistry had primarily dealt with a narrow area of kinetics and mechanisms of reactions in solution. It created an intellectual framework for much of current chemistry. More recently it has been strength-

ened by diversifying into the interstices between organic chemistry and other fields, including such areas as solid state and supramolecular chemistry, gas phase reactions, computational chemistry and biochemistry.

The Commission believes it is now timely to assess the future of physical organic chemistry and to look to where the opportunities exist for future research. The barriers between the various fields of chemistry are disappearing, and this may be a reason to reorganize the entire field along conceptual lines. This is a responsibility that IUPAC is uniquely suited to assume. The Commission has therefore solicited expert opinions about the future of this interdisciplinary field. Opinions were requested from a diverse group of leaders in chemistry, known for their creativity and not necessarily identified as physical organic chemists. Instead, they were chosen from those who have contributed to physical organic chemistry, broadly viewed, or who utilize the results of physical organic chemistry. Authors were asked to look to the future, rather than to emphasize past research contributions, although they were encouraged to review the previous development of their field if that would help put the future prospects in perspective.

Contributions are published from: T.T. Tidwell, Department of Chemistry, University of Toronto, Toronto, Ontario, Canada, and Chair of the IUPAC Commission on Physical Organic Chemistry 1993–1997; E.M. Arnett, Department of Chemistry, Duke University, Durham, North Carolina, USA; R. Breslow, Department of Chemistry, Columbia University, New York, USA; F. Cacace, Dipartimento di Studi di Chimica e Tecnologia delle Sostanze Biologicamente Attive, Università di Roma 'La Sapienza', Rome, Italy; J.B.F.N. Engberts, Department of Organic and Molecular Inorganic Chemistry, University of Groningen, Groningen, the Netherlands; M.A. Fox, Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, Texas, USA; K.N. Houk and J.K. Lee, Department of Chemistry and Biochemistry, University of California, Los Angeles, California, USA; K.U. Ingold, Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Ontario, Canada; A.R. Katritzky, M. Karelson and V. S. Lobanov, Florida Center of Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, Florida, USA; E. M. Kosower, Biophysical Organic Chemistry Unit, School of Chemistry, Tel-Aviv University, Tel-Aviv, Israel; M. Lahav, Department of Materials and Interfaces, The Weizmann Institute of Science, Rehovot, Israel; T. Mukaiyama, Department of Applied Chemistry, Faculty of Science, Science University of Tokyo, Tokyo, Japan; O. M. Nefedov and M. P. Egorov, N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia; G. A. Olah, Loker Hydrocarbon Research Institute and Department of Chemistry, University of Southern California, Los Angeles, California, USA; J. D. Roberts, Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena, California, USA; S.-M. Savéant, Laboratoire d'Electrochimie Moléculaire de l'Universit é Denis Diderot, Paris, France; D. Schröder, C. Heinemann, W. Koch and H. Schwarz, Institut für Organische Chemie der Technische Universität Berlin, Berlin, Germany; A. Streitwieser, Department of Chemistry, University of California, Berkeley, California, USA; J. Vogt and D. Bellus, Ciba-Geigy, Corporate Research Units, Marly and Basel, Switzerland; F.H. Westheimer, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts, USA; and A. Yamamoto, Department of Applied Chemistry, School of Science and Engineering, Waseda University, Tokyo, Japan.

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry.*

Basic terminology of stereochemistry (IUPAC Recommendations 1996)

Synopsis

This is a glossary of the more important, and most widely-used, stereochemical terms. It extends the list of those defined in the IUPAC Nomenclature of Organic Chemistry, Section E: Stereochemistry (Recommendations 1974) and includes some terms from the Glossary of Terms used in Physical Organic Chemistry (Recommendations 1994). Additional terms have been added from inorganic and macromolecular chemistry. Some misleading terms are included together with guidance on correct usage or acceptable alternatives.

This Report was prepared for publication by G. P. Moss (Department of Chemistry, Queen Mary and Westfield College, Mile End Road, London, E1 4NS, UK) for the Commissions on Nomenclature of Organic Chemistry (III.1) and Physical Organic Chemistry (III.2) of the Organic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1996, ***68****, 2193–2222.*

Glossary of terms used in photochemistry (IUPAC Recommendations 1996)

Synopsis

A provisional version of this Glossary was published in the period 1983–1984 in the Newsletters of the European Photochemical Association, the Inter-American Photochemical Society, and the Japanese Photochemical Association. The first edition of the Glossary of Terms Used in Photochemistry, prepared for publication in the Commission by S.E. Braslavsky and K.N. Houk, was published in 1988 (*Pure Appl. Chem.* 1988, **60**, 1055–1106) and has since been incorporated in the Handbook of Organic Photochemistry Vol II, J.C. Scaiano Ed., CRC Press, Boca Raton, 1989, and in Photochromism: Molecules and Systems, H. Dürr and H. Bouas-Laurent Eds., Elsevier Science Publishers, 1990. In this second edition a number of minor errors encountered in the first edition have been corrected and the Glossary has been expanded to incorporate terms related to (photoinduced) electron transfer processes.

This Report was prepared for publication by J. W. Verhoeven (Laboratory of Organic Chemistry, University of Amsterdam, Nieuwe Achtergracht 129, 1018 WS Amsterdam, the Netherlands) for the Commission on Photochemistry of the Organic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1996, ***68****, 2223–2286.*

Glossary of basic terms in polymer science (IUPAC Recommendations 1996)

Synopsis

In 1974, the Commission on Macromolecular Nomenclature published a document entitled Basic Definitions of Terms Relating to Polymers (1974) (*Pure Appl. Chem.* 1974, **40**, 479–491). These definitions have been the foundation for the Commission's work and, building on this basis, the Commission has developed a number of further nomenclature documents. The vast majority of terms in the basic document serve their purpose well. Progress in polymer science and the need for new definitions, the proper wording of which would have been incompatible with some of the basic terms, made it increasingly apparent that some change was needed in the basic terms. Approximately 20 years after the publication of the first document, the Commission now issues a revised and enlarged set of basic terms.

This report was prepared for publication by a Working Group consisting of A.D. Jenkins (UK), P. Kratochvíl (Czech Republic), R.F.T. Stepto (UK) and U.W. Suter (Switzerland) for the Commission on Macromolecular Nomenclature of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1996, ***68****, 2287–2311.*

Definitions of terms relating to degradation, aging, and related chemical transformations of polymers (IUPAC Recommendations 1996)

Synopsis

Chemical reactions of polymers are very important from the points of view of chemical modifications of polymers to improve properties and changes in structure and physico-chemical properties in the course of synthesis, processing, processing, application or the action of chemicals or micro-organisms. However, terminology has developed only on *ad hoc* bases in different professional communities. Hence this document presents an alphabetical list of terms relating to degradation, aging and related chemical transformations of polymers, and defines a self-consistent terminology for the field to aid communication and avoid confusion. Some of the general definitions are modified by one or more prefixes or adjectives describing type or cause. Definitions of basic terms, such as aging, degradation and stability, have notes appended relating to specific cases. Adjective-modified terms that are frequently used by themselves are defined separately.

This Report was prepared for publication by a Working Group consisting of K. Hatada (Japan), R.B. Fox (USA), J. Kahovec (Czech Republic), E. Maréchal (France), I. Mita (Japan) and V. Shibaev (Russia) for the Commission on Macromolecular Nomenclature of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1996, ***68****, 2313–2323.*

Preservation and utilization of natural biodiversity in context of search for economically valuable medicinal biota (Technical Report)

Synopsis

Natural products remain excellent sources of leads in the search for novel medicaments for the treatment of diseases. The largest underexplored source of such materials lies in tropical and subtropical regions. In these areas a long tradition of ethnobotanical medicine often exists with which to guide laboratory experimentation, but the finds, equipment and necessary expertise are often lacking. The divergence between availability and the means to develop provides the basis for significant disagreements over the value to be placed on each party's contribution and represents a factor which inhibits the development of these materials. Various scientific societies, governmental agencies, industries, groups and individuals have advanced their views, but no amicable consensus has emerged. IUPAC has considered a number of declarations on the subject, particularly the Manila Declaration of 1992 and the Melaka Accord of 1994, which are reproduced in an appendix, and has made several recommendations for participants promulgating declarations and enacting legislation. This position paper sets forth IUPAC's views for the guidance of its members and affiliated organizations.

*This Report was prepared for publication by P.R. Andrews (Australia), R. Borris (USA), E. Dagne (Ethiopia), M.P. Gupta (Panama), L.A. Mitscher (USA), A. Monge (Spain), N.J. de Souza (India) and J.G. Topliss (USA) for the Section on Medicinal Chemistry. The full details are to be found in Pure Appl. Chem. 1996, **68**, 2325–2332.*

General features of contracts for natural product collaborations (Technical Report)

Synopsis

Many scientists in developing countries are interested in orderly development on an equitable basis of economically useful discoveries based upon research on indigenous natural products. Availability of funds and technical expertise in the country of origin is often a limiting factor. Cooperation with individuals and organizations possessing these is frequently a practical necessity for the work to go forward. Inexperience in patent and legal matters as well as perceived differences in comparative power are often found to be inhibitory. The discussion by IUPAC is intended to be helpful in such cases by setting forth the elements which are commonly present in collaborative contracts. This material was developed by considering a dozen such contracts in present effect between persons from several different countries of origin and firms based in Europe and the USA. This paper is not a contract, but indicates the elements usually present and the negotiable items which need to be settled amicably.

*This report was prepared for publication by P.R. Andrews (Australia), R. Borris (USA), E. Dagne (Ethiopia), M.P. Gupta (Panama), L.A. Mitscher (USA), A. Monge (Spain) and N.J. de Souza (India) for the Section on Medicinal Chemistry. The full details are to be found in Pure Appl. Chem. 1996, **68**, 2333–2337.*

Atomic weights of the elements 1995 (Technical Report)

Synopsis

The biennial review of atomic weight determinations and other cognate data has resulted in changes for the standard atomic weight of the following 21 elements: boron, carbon, fluorine, sodium, aluminium, phosphorus, scandium, manganese, cobalt, arsenic, rhodium, caesium, cerium, praseodymium, europium, terbium, holmium, thulium, platinum, gold and bismuth. An annotation for potassium has been changed in the Table of Standard Atomic Weights. To eliminate possible confusion in the reporting of relative lithium isotope-ratio data, the Commission on Atomic Weights and Isotopic Abundances recommends that such data be expressed using $^{7}Li/^{6}Li$ ratios and that reporting using $^{6}Li/^{7}Li$ ratios be discontinued. Because relative isotope-ratio data for sulfur are commonly being expressed on non-corresponding scales, the Commission recommends that such isotopic data be expressed relative to VCDT (Vienna Canon Diablo Troilite) on a scale that $^{34}S/^{32}S$ of IAEA-S-1 silver sulfide is 0.9997 times that of VCDT. Many elements have a different isotopic composition in some non-terrestrial materials. Some recent data on oxygen are included.

*This Report was prepared for publication by T. B. Coplen (US Geological Survey, Reston, Virginia 20192, USA) for the Commission on Atomic Weights and Isotopic Abundances of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1996, **68**, 2339–2359.*

Reporting of relative sulfur isotope-ratio data (Technical Report)

Synopsis

To eliminate possible confusion in the reporting of sulfur isotope-ratio data, the Commission on Atomic Weights and Isotopic Abundances recommends that relative $^{34}S/^{32}S$ ratios of all sulfur-bearing substances be expressed on the VCDT (Vienna Canon Diablo Troilite) scale, defined by assigning a $\delta^{34}S$ value of –0.3‰ exactly (relative to VCDT) to the silver sulfide reference material IAEA-S-1. Reporting of sulfur isotope-ratio analyses relative to CDT (Canon Diablo meteorite) should be discontinued.

This Report was prepared for publication by H.R. Krouse (University of Calgary, Calgary, Alberta T2N 1N4, Canada) and T.B. Coplen (US Geological Survey, Reston, Virginia 20191, USA) for the Commission on Atomic Weights and Isotopic Abundances of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, ***69****, 293–295.*

A statistical overview of standard (IUPAC and ACS) and new procedures for determining the limits of detection and quantification: Application to voltammetric and stripping techniques (Technical Report)

Synopsis

Traditional methods for determining the limit of detection (LOD) and the limit of quantification (LOQ), based on the IUPAC and ACS definitions, often are unsatisfactory. Consequently, a new, simple and statistically correct way of obtaining both the LOD and LOQ values has been derived and compared to commonly used methods. The new Upper Limit Approach, ULA, calculates the upper confidence limit of an individual blank signal using a critical value of the t-distribution and standard error of estimate (residual standard deviation) of regression. The uncertainty of the calibration plot position, its intercept and the mean blank signal are taken also into consideration. The proper choice of calibration model and calibration design are also discussed in detail. An improved derivation of the signal value relevant to the LOQ is based on the use of the same significance level needed for defining the LOD. The concepts developed in this paper have been applied to the determination of cadmium by five common techniques of electrochemical trace analysis (DC tast polarography, differential pulse polarography, linear sweep stripping voltammetry, differential pulse stripping voltammetry and potentiometric stripping analysis) under equivalent (as possible) conditions. The lowest LOD and LOQ values, obtained by the new reliable ULA method, were 1.0×10^{-9} mol/L and 3.1×10^{-9} mol/L Cd, respectively, for differential pulse stripping voltammetry and significance level $\alpha = 0.01$. The relevant LOD and LOQ values for $\alpha = 0.05$ are 6.6×10^{-10} mol/L and 2.0×10^{-9} mol/L Cd, respectively. Potentiometric stripping analysis provided similar results.

This Report was prepared for publication by Jan Mocak, A.M. Bond and S. Mitchell (School of Chemistry, La Trobe University, Bundoora, Victoria 3083, Australia) and G. Scollary (School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, ***69****, 297–328.*

Stability constants for alpha-hydroxycarboxylic acid complexes with protons and metal ions and the accompanying enthalpy changes. Part I: Aromatic ortho-hydroxycarboxylic acids (Technical Report)

Synopsis

Stability constants for different aromatic ortho-hydroxycarboxylic acid complexes in aqueous solutions with protons and metal ions published between 1970 and the end of 1993 have been critically evaluated. For comparison, some data published earlier than 1970 are included. In some cases, data obtained in aqueous solutions are compared to those obtained in solvent mixtures such as water-ethanol or water-DMSO. In addition to the stability constants, the enthalpy changes of those systems which are available are included.

This report was prepared for publication by Lauri H.J. Lajunen (Department of Chemistry, University of Oulu, SF-90570 Oulu, Finland), Roberto Portavnova (Department of Chemistry, University of Udine, I-33100 Udine, Italy), Juha Piispanen (Department of Chemistry, University of Oulu, SF-90570 Oulu, Finland) and Marilena Tolazzi (Department of Chemistry, University of Udine, I-33100 Udine, Italy) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, ***69****, 329–381.*

New Publications

IUPAC Solubility Data Series

The Solubility Data Project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from independent sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values and compiled data sheets are published on consecutive pages.

Volume 63: Metals in Liquid Alkali Metals Part I: Be to Os

Volume 64: Metals in Liquid Alkali Metals Part II: Co to Bi

Volumes 63 and 64, edited by Hans Ulrich Borgstedt and Cezary Guminski, contain the first and second parts of the collection of evaluated experimental solubility data of about 70 metallic elements in five alkali metal solvents (Li, Na, K, Rb, Cs). The systems were ordered following the IUPAC-accepted long periodic table for the solutes and following the atomic number for the solvent elements. The mutual binary systems of the alkali metals themselves are treated briefly in the first pages of Volume 63. They are characterized by either complete miscibility in some of the systems or large miscibility gaps in others. They are presented for general information in the form of assessed phase diagrams.

Solubility data of metals in liquid alkali metals are widely spread over journals, congress proceedings, rare reports of several organizations in France, Germany, the UK and the US, and unique literature which has appeared only in the Russian language. The first publications concerned with binary systems of alkali metals with other metallic elements appeared at the end of the last century; the literature is covered inclusively up to 1994. *Chemical Abstracts, Nuclear Science Abstracts* and *Atom Index* were used as primary sources for the reference search of solubility data. It was soon discovered that the keyword *solubility* was not sufficient to extract complete solubility information from the corresponding literature. Therefore entries related to this subject were also inspected. Since none of the reviews was sufficiently complete, it was decided to collect and assess anew all experimental results available. If not otherwise stated, the data sheets were prepared directly from the original papers. Any secondary sources were used only sporadically if original reports were not accessible.

Volume 65: Copper(I) Halides and Pseudohalides

Volume 65, edited by James J. Fritz and Erich Königsberger, describes the solubility properties of the halides and pseudohalides of copper(I) in both aqueous and non-aqueous media. The salts considered are CuCl, CuBr, CuI, CuSCN, CuSeCN, CuCN, Cu_2CN_2 and CuN_3, and in addition the double or other complex salts which can be formed when the simple salts dissolve in suitable media. The information presented is based on a thorough literature search through 1988. Media for which solubility data have been reported include both pure solvents and solutions containing other substances which promote dissolution of the cuprous salt. The properties considered in this book include the solubilities themselves, phase diagrams where observed and such thermodynamic properties as may aid in treatment of the solubility data. Since in a number of systems double salts were produced upon dissolution of a cuprous halide, information is provided on the double salts which have been produced from the various halides. Recommended values of solubility are given where the available data appear reliable enough to make this feasible.

Volumes 63, 64 and 65 of the IUPAC Solubility Data Series (ISSN 0191-5622) were published in June, September and December 1996 by Oxford University Press, Oxford, UK. Negotiations to contract a new publisher in 1997 by the Commission on Solubility Data are at an advanced stage. Details will be announced in due course.

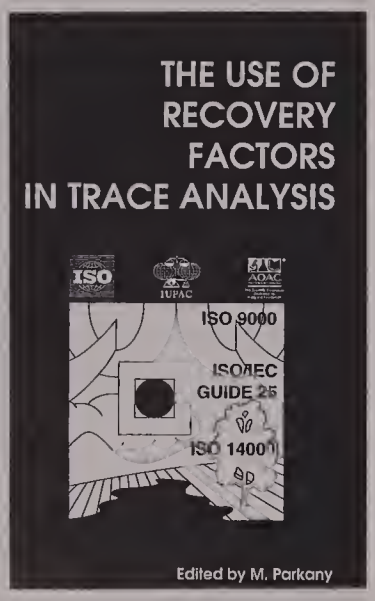
Medicinal Chemistry: Today and Tomorrow

Medicinal chemistry is an interdisciplinary science covering a broad range of subjects, but with chemistry as its core and the goal of producing effective new pharmaceuticals. This book presents the edited proceedings of the AFMC International Medicinal Chemistry Symposium held in Tokyo, Japan, 3–8 September 1995. The symposium was organized by the Pharmaceutical Society of Japan on behalf of the Asian Federation for Me-

dicinal Chemistry (AFMC). It consisted of eight plenary lectures, 40 invited lectures in 13 sessions, and 185 discussions stimulated by posters. Although research on medicinal chemistry is broad and various, the plenary lecturers are all leading scientists with outstanding achievements in their own fields. Medicinal chemistry has seen remarkable advances in recent years, and *Medicinal Chemistry: Today and Tomorrow* provides an overview of the state of the art.

Medicinal Chemistry: Today and Tomorrow. Proceedings of the AFMC International Medicinal Chemistry Symposium held in Tokyo, Japan, 3–8 September 1995. Edited by Mikio Yamazaki. Published on behalf of IUPAC by Blackwell Science, Osney Mead, Oxford OX2 0EL, UK, 1997. Price: GBP 49.50. ISBN 0-632-04272-9.

The Use of Recovery Factors in Trace Analysis



This book contains the proceedings of the Seventh International Harmonization Symposium on a Protocol for Recovery Factors held in Orlando, Florida, on 4–5 September 1996, under the sponsorship of IUPAC, ISO and AOAC International. The correct implementation of the ISO 14000 series of international standards is entirely dependent on valid measurements, which in turn require the correct approach to recovery factors—yet at present there is no international standard or guide to the correct use of recovery factors. This means that it is problematic to obtain a real picture of whether and when the use of recovery factors is forbidden, tolerated, encouraged or required; often the choice is left to the analyst in charge. The lectures in these proceedings review the present situation and offer practical solutions based on analysts' experiences. This book will form the basis for a document on conformity assessment to standards proposed by IUPAC, ISO, AOAC and Codex Alimentarius Commission.

The Use of Recovery Factors in Trace Analysis. Edited by M. Parkany, International Organization for Standardization, Geneva. Published by The Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF, UK, 1996. ISBN 0-85404-736-0.

Nomenklatur der Organischen Chemie: Eine Einführung

The 'Blue Book' *Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993*, prepared for publication by R. Panico, W. H. Powell and Jean-Claude Richer and published by Blackwell Scientific Publications in 1993, has been translated into German. The German edition, *Nomenklatur der Organischen Chemie: Eine Einführung,* prepared under the auspices of the Gesellschaft Deutscher Chemiker in cooperation with the Neuen Schweizerischen Chemischen Gesellschaft and the Gesellschaft Österreichischer Chemiker, is published by VCH, D-69451 Weinheim, Germany, 1997. Price DM 168. ISBN 3-527-29327-2.

IPCS Health and Safety Guides

Two newly published guides in the IPCS (International Programme on Chemical Safety) Health and Safety series are:

No.102: Thallium and Thallium Compounds Health and Safety Guide. A companion volume to Environmental Health Criteria 182: Thallium. ISBN 92 4 151102 8.

No.103: White Spirit (Stoddard Solvent) Health and Safety Guide. A companion volume to Environmental Health Criteria 187: White Spirit. ISBN 92 4 151103 6.

Both guides are published by the World Health Organization for the International Programme on Chemical Safety (a collaborative programme of the United Nations Environment Programme, the International Labour Organisation and the World Health Organization) and produced within the framework of the Inter-Organization Programme for the Sound Management of Chemicals.

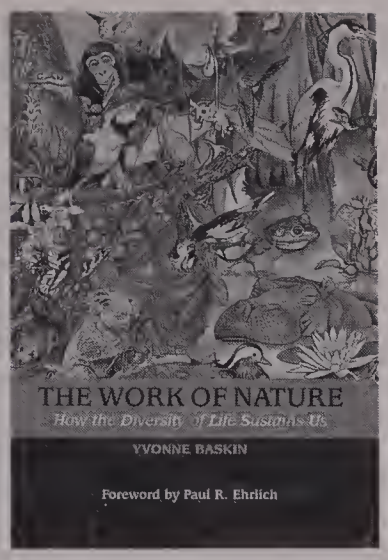
New SCOPE publications

Three new publications on SCOPE (Scientific Committee on Problems of the Environment) projects have recently been published. They are:

The Work of Nature: How the Diversity of Life Sustains Us

This book summarizes and explains key findings from the ecological sciences on the practical consequences of declining biodiversity on ecosystem health and functioning. In 1991, SCOPE launched a programme specifically to review and evaluate all scientific literature relevant to the subject of ecosystem functioning. This brought together specialists in the major ecosystems of the earth, including coral reefs, tropical forests, deserts and tundra, first in a series of ecosystem-specific workshops and then as a single group to compare results

from their respective systems and to assess similarities and differences. Subsequently, the United Nations Environment Programme launched a Global Biodiversity Assessment, which incorporated and expanded the SCOPE project and represented the first time the significance of biodiversity loss on ecosystem functioning had been addressed. Science journalist Yvonne Baskin was then commissioned by the SCOPE Scientific Steering Committee to bring the project's findings to a broad audience. The result is *The Work of Nature,* the first book of its kind to distil and bring to life the work of the world's leading ecologists.



The Work of Nature: How the Diversity of Life Sustains Us. By Yvonne Baskin; Foreword by Paul R. Ehrlich. Published by Island Press, 1718 Connecticut Avenue NW, Suite 300, Washington, DC 20009, USA, 1997. ISBN 1-55963-519-3 (clothbound).

Functional Roles of Biodiversity: A Global Perspective

This book addresses a number of important issues including whether biodiversity has a significant role to play in system processes, how system stability and resistance are affected by species diversity, and how global change will affect these relationships. In addressing these questions, this volume of the SCOPE series synthesizes knowledge of the functional role of biodiversity, bridging the gulf between research in population ecology and ecosystem ecology, and also develops the basis for an experimental programme for inclusion into the International Geosphere Biosphere Programme.

Functional Roles of Biodiversity: A Global Perspective. Edited by Harold A. Mooney, J. Hall Cushman, Ernesto Medina, Osvaldo E. Sala and Ernst-Detlef Schulze. Published by John Wiley & Sons, Baffins Lane, Chichester, West Sussex PO19 1UD, UK, 1996. ISBN 0-471-95601-5.

Global Change: Effects on Coniferous Forests and Grasslands

To improve understanding of ecosystem responses to climate change, SCOPE sponsored a project on the effects of climate change on production and decomposition processes in coniferous forests and grasslands (temperate and tropical) emphasising carbon fluxes and pools. The project had three objectives: a critical assessment of current understanding of the effects of such climate change; a review of extant forest and grassland ecosystem models and an evaluation of their usefulness for studies of the effects of climate change on production and decay processes; and the development of diagnostic and predictive models to describe the effects of climate change on forests and grasslands and to work at multiple space and time scales, so as to permit better extrapolation and analysis of climate change scenarios. *Global Change: Effects on Coniferous Forests and Grasslands* provides critical baseline information, modelling strategies, and identifies future research strategies on coniferous forests and grasslands, which will be relevant for basic and applied research.

Global Change: Effects on Coniferous Forests and Grasslands. Edited by A.I. Breymeyer, D.O. Hall, J.M. Melillo and G.I. Ågren. Published by John Wiley & Sons, Baffins Lane, Chichester, West Sussex PO19 1UD, UK, 1996. ISBN 0-471-96837-4.

Laboratory Diagnosis of Group A Streptococcal Infections

This manual provides a detailed guide to virtually all procedures commonly required for the laboratory evaluation of group A streptococcal infections. It includes advice not only on bacteriological methods, but also on serological evaluations and streptococcal antibody tests. Descriptions are also included of other important techniques, such as the preparation of antisera for streptococcal stereotyping, many of which cannot be purchased commercially. The methods described are a compilation of the extensive experience in the two reference laboratories where the authors work, but procedures and suggestions from the published literature are also included.

Laboratory Diagnosis of Group A Streptococcal Infections. By Dwight R. Johnson and Edward L. Kaplan (WHO Collaborating Centre for Reference and Research on Streptococci, Minneapolis, MN, USA) and Jaroslav Sramek, Ruth Bicova, Jiri Havlicek, Helena Havlickova, Jitka Motlova and Paula Kriz (WHO Collaborating Centre for Reference and Research on Streptococci, Prague, Czech Republic), published by the World Health Organization, Geneva, 1996, vii + 111 pages (English; French and Spanish in preparation). Price: CHF 32.-/ USD 28.80; Price in developing countries: CHF .22.40. ISBN 92 4 154495 3.

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most recent list of the national/regional centres appeared in *Chemistry International* 1995, **17**, 141.

Glossary of Terms Used in Medicinal Chemistry

A Working Party of the IUPAC Section on Medicinal Chemistry has prepared a glossary consisting of about 100 commonly employed terms which can be considered of particular interest to the medicinal chemistry community. The aim is to provide in a single document a consistent terminology and concise definition of terms covering the various aspects of medicinal chemistry. The glossary has been compiled in part from definitions proposed by the Working Party and in part from well-accepted definitions taken from the literature but which were sometimes published in journals or books that may not be readily accessible.

Some definitions taken from the *Glossary for Chemists of Terms Used in Biotechnology* (*Pure Appl. Chem.*, 1992, **64,** 143–168) were also included; they are identified by an asterisk*. Others, which appear in the *Glossary on Computational Drug Design* (to be published in 1997 in *Pure Appl. Chem.*), are identified by a double asterisk**.

Comments on these recommendations are welcome and should be sent by 30 September 1997 to: Prof. C.G. Wermuth, Faculté de Pharmacie, Université Louis Pasteur, Strasbourg, France.

Revised Section F: Natural Products and Related Compounds

The nomenclature of natural products has suffered from much confusion, mostly for historical reasons. The isolation of new substances in the early days of the science generally preceded characterization by a lengthy period. Thus these compounds were often assigned trivial names that gave no indication of the structure of the molecule and were often found afterwards to be misleading. The IUPAC Commission aims to unite as far as possible all the specialists reports into a single set of recommendations that can be applied to most areas of natural product chemistry. Provisional recommendations were prepared and published as Section F of the IUPAC Organic Nomenclature Rules, first in 1976, and then in the 1979 edition of the Rules.

The revision of these provisional recommendations is now complete and presented under the title *Revised Section F: Natural Products and Related Compounds.* Two chapters describe and exemplify the rules to deal with biologically based trivial names, semisystematic names and fundamental parent structures. The following chapters deal with skeletal modifications, applications of different types of nomenclature to the parent structures ('a' replacement nomenclature, fusion nomenclature, bridging, substantive nomenclature). A chapter on the variation of the degree of hydrogenation is included. The final chapter deals with stereochemistry.

The document includes an appendix presenting stereoparent structures and numbering of 72 alkaloids, 15 steroids, 45 terpenoids and eight miscellaneous compounds.

Comments on these recommendations are welcome and should be sent by 30 September 1997 to: Prof. H.-A. Favre, Département de Chimie, Université de Montréal, BP 6128, Succursale A, Montréal, Quebec H3C 3J7, Canada.

Conference Report

A Sustainable Environment: National and International Perspectives

Organized by Prof. Pieter Steyn of IUPAC's newly established Division of Chemistry and the Environment and held at the CSIR Conference Centre in Pretoria, South Africa, on 5 December 1996. The event attracted 175 delegates, representing senior managers from the public and private sectors, environmental scientists, teachers and students.

The symposium addressed perspectives on how to sustain the environment, and the role that chemistry could and should play. Many different issues were addressed, ranging from intricate chemistry to industrial waste management. The morning sessions dealt with environmental pollution resulting from human activities or nature itself. After lunch, interesting views on tropospheric ozone and the movement of pollutants in lakes were raised. During the afternoon session speakers presented the new approaches and attitudes required to solve the environmental problems facing industry, government and society in general.

In the welcoming address Dr Junshi Miyamoto, President of IUPAC's Division of Chemistry and the Environment (DCE), stated that the progress of science should foremost benefit humanity, for example by producing enough good quality food and medicine, without harming the environment. The emphasis should be on efficient production to increase yield and minimize waste. To attain these ideals more fundamental research on new materials, ranging from less polluting power generators to high yielding crop species, is required. In order to achieve this, IUPAC, and specifically the DCE, intend to be major players.

Dr Khotso Mokhele, President of the Foundation for Research Development, the body in South Africa mainly responsible for research funding at universities, sees South Africa as a microcosm of the challenges facing the world. According to the Bill of Rights, every South African has a right to an environment that is not harmful and is protected for present and future generations. To attain this, South Africa has adequate expertise on environmental management, and has recently published two green papers on environmental policies. However, currently it lacks sufficient qualified experts to implement these suggestions. The challenge is thus to translate these policies into successful action plans, keeping the inseparability of the environment and economy in mind, while acknowledging human resources. Dr Mokhele further stressed the important role of education, especially mathematics and science, in attaining and maintaining a sustainable environment.

Prof. Werner Klein from the Fraunhofer Institut für Umweltchemie und Ökotoxikologie, Germany, addressed the ecotoxicological assessment of pollutants. He maintained that it would be ideal if all potential risk substances from all technological activities were assessed by a systematic technologically oriented approach. There are different levels in a tiered approach to risk assessment, starting with the identification of potential hazards based on the substance's intrinsic properties. The next step is the classification and labelling of the substance. Finally, after hazard and risk assessment, the actual risk can be established. Only then is it possible to implement risk management, monitor product use and/or possibly substitute hazardous components. Unfortunately, current surveillance programmes

Gathered during one of the tea breaks are: Prof. Pieter Steyn of the Centre for Chemistry at the University of Potchefstroom and organizing chairman of the symposium, Dr Junshi Miyamoto, President of the DCE of IUPAC, and FRD President Dr Khotso Mokhele, who delivered the opening address.

are not nearly adequate to assess the vast number of chemical products, and much research is still required.

Dr Terry Roberts, of JSC International, UK, spoke about the environmental behaviour of agrochemicals. Since agrochemicals are purposefully introduced into the environment, their use is highly regulated and the setting of specific requirements has received much attention over the past few years. Different assessment schemes (EPA, EU, OECD) have been recommended to determine the fate of these chemicals in the environment. IUPAC has made recommendations in this area with an approach that involves three levels of testing: exploratory, verification and surveillance. For the future it will be increasingly important to complement laboratory and field data with computer models, and harmonization of test guidelines. Finally, it is essential to integrate information on all contributing factors including pesticide behaviour, cropping, soils, climate and geography.

In his lecture on hazardous chemicals in oils, fats and derivatives, Dr Albrecht Dieffenbacher, of the Nestlé Research Center, Switzerland, maintained that hazardous chemicals can potentially be introduced into oils and fats during all stages of production, harvesting, refining and handling. Collaborative studies have been undertaken by IUPAC and related bodies, which show that skilled analysts are needed to detect and if possible remove contamination. The intensive research and regulatory actions have led to much safer products reaching the consumer.

Dr Pieter Thiel, Chairperson of the IUPAC Commission on Food Chemistry, discussed the role of natural toxins, mycotoxins and phytotoxins in environmental pollution. Toxins in the environment can be of man-made or natural origin. However, the effects of natural toxins are usually underestimated, especially where people depend on one food source, such as maize in Africa. Natural toxins are formed by various organisms including algae, fungi, bacteria, plants and animals. Their toxicities differ vastly, for example the relative carcinogenic potency of the naturally occurring aflatoxins my be 1000 times higher than the toxicity of man-made synthetic chemicals. There are two important groups of toxins formed by fungi, aflatoxins and fumonisins. The estimated tolerable daily intake of fumonisin is 0.8 μg/kg/day. This is easily met in Germany where the daily intake does not exceed 0.05 μg/kg/day. However, in the Transkei in South Africa the fumonisin exposure could be as high as 11.0 μg/kg/day. This goes to show that the risk of these and other toxins depends not only on their intrinsic toxicity but also on the exposure level to humans. This presentation has illustrated that natural toxins cannot be ignored when dealing with environmental pollution.

In his second presentation Prof. Klein discussed the remediation of hazardous waste sites, an issue that is currently attracting much attention. Hazardous waste sites have different origins, such as mining, industry and military, and different treatment technologies are available, for example incineration, washing and bioremediation. Several criteria, including economic factors, size of the site, type of pollutant and intended future use of the site, need to be considered when choosing a treatment method. An interesting example of remediation presented showed the use of heavy metal contaminated soil for brick fabrication. However, further validation is essential to establish the safety of the residual toxicants in spite of fixation. Problems that are still encountered with remediation involve the determination of target values, the safety of immobilization and remediation control.

Rufus Maruma, of Waste-Tech, South Africa, spoke on industrial waste management. According to Dr Pallo Jordan, South African minister of environmental affairs, South Africa does not have a very good track record on environmental issues. Very little is known of the type, amount and disposal of waste produced in the country. In addition, many waste sites are not appropriately supervised and are frequently in an unacceptable condition. To rectify this, Mr. Maruma sees the need for collaboration between industry and government, implying that industry should manage those activities that government cannot, such as hazardous waste management. The priority for waste management should be waste avoidance, waste recycling, waste treatment and only then waste disposal. Waste can be disposed of by incineration, landfilling, pumping into the sea, in sewers and deep wells. However, landfilling is the most cost-effective means of large-scale disposal in South Africa.

Dr Bob Scholes, a CSIR fellow, alluded to the savannas as a source of ozone-forming trace gases. Every year during August/September a large cloud of ozone appears in the troposphere over the west coast of Africa. This phenomenon was initially associated with veld fires (biomass burning). Dr Scholes studied some precursors, including nitric oxide, methane and carbon monoxide, to verify the origin of the ozone cloud and found that the precursors originate from pyrogenic (fire), biogenic (soil) or industrial (exhaust fumes) sources. The effect of fire and moisture, especially the first rains after the winter, on the emission of ozone precursors was evaluated; this showed that the role of fire on ozone formation was overestimated. The investigations clearly showed that the seasonal ozone maximum has a mixed and complex origin.

Prof. Kobus Pienaar, of Sasol's Centre for Chemistry, has also investigated tropospheric ozone. He spoke on the role of the African continent in tropospheric ozone pollution. Being a pollutant (unlike the ozone layer in the

stratosphere) the increased ozone concentration in the troposphere is a matter of great concern. The ozone in the troposphere is formed by the oxidation of hydrocarbons. However, the presentation showed that ozone could also act as a detergent of the troposphere, forming hydroxyl radicals that are highly reactive towards carbon monoxide, methane and hydrocarbons, breaking them down to carbon dioxide and formaldehyde. These reactions are pH and water dependent. Studies have further shown that the ozone concentration in the northern hemisphere is much higher than the average ozone pollution over Africa. It was with this in mind that Prof. Pienaar concluded that the ozone over Africa played an important role by acting as a detergent as it 'washes for the world'.

Prof. Jacques Buffle, of the Université de Geneve, Switzerland, addressed the physicochemical and analytical aspects involved during the transport of trace compounds by colloids in aquatic systems. The presentation dealt with the different approaches that could be used when studying or modelling the circulation of pollutants in a lake. He stated that pollutants in a lake have two paths that they can follow, either being absorbed on a colloid to form a sedimentation layer or being washed into the river. Most models lack either biophysical or macroscopic aspects, but it is vital that both facets are included. Studies should be conducted on macroscopic, microscopic and molecular levels which can be linked by mathematical modelling. This biophysical chemistry modelling of the environment can then lead to environmental monitoring and finally environmental management.

Dr Junshi Miyamoto, of Sumitomo Chemical, Japan, introduced delegates to the fascinating research and development of agrochemicals in the era of sustainable development. The development of novel agrochemicals aims to reduce the shortcomings of their predecessors on the environment, for example persistence and accumulation in soil and the food chain with adverse effects on humans and wildlife. The current approach to developing new agrochemicals makes use of integrated disciplines (computer modelling, biology, chemistry and biochemistry) and optimization processes. One example of this approach is the testing of biologically active natural products as possible new pesticides. However, the research is tedious as only one in 10 000 compounds successfully meets the requirements, given the many facets that have to be borne in mind, such as insect resistance and herbicide tolerant varieties.

Dr Laurraine Lotter, of the Chemical and Allied Industries Association, provided insights on Responsible Care, a key element in the approach of the chemical industry to sustainable development. Responsible Care is an international initiative supported by industry and committed to doing the 'right thing'. This approach entails employee education, pollution prevention, waste minimization, resource conservation, emergency preparedness and rehabilitation of the environment. Member companies are 'open' about their activities and try to integrate environmental issues into business planning, while continuously attempting to improve and maintain good manufacturing practice. In 1994, this plan was introduced to South Africa. To date, 104 companies have taken the first step of committing themselves to Responsible Care principles.

Prof. Jim Petrie, of the University of Cape Town, also sees technology as a driver for change towards a sustainable society. He maintained that one of the key problems facing industry is the balance between economical development and preventive environmental management. Therefore clean technology could be defined as the provision of services and products whilst consuming fewer resources and generating less environmental impact, but still maintaining economical competitiveness. For a total life cycle assessment it is important to be aware of the environmental impact of resource extraction, product use and waste disposal. Furthermore, it is important to minimize not only the waste, but also the environmental impact, which should influence the decision process. It can therefore be said that environmental management should be based on a multicriterion decision analysis. Prof. Petrie concluded that, with efficient technology, environmental management systems and life cycle analysis in place and an innovative approach to continual improvement, a sustainable competitive advantage can be attained.

After a long and meaningful day, Dr Arie Geertsema, of Sastech Research and Development, concluded that there was a need to correct the short-sightedness of the past, where actions were mostly profit oriented. Yet the symposium has clearly shown industry's increased environmental awareness. However, environmental sustainability is not only the responsibility of industry and government, but that of society as a whole. Through awareness, society should not only assure that a factual base is provided and communicated to decision makers, but also become involved in the decision making process. In South Africa the necessary new policies are in place, the next step should be appropriate actions, ensuring that 'we not only do the right things, but that we do the right things correctly'.

In summary, this symposium provided both an excellent international perspective and very valuable insight into the research activities and particular issues facing South Africa in striving for a sustainable environment.

Prof. Pieter Steyn and Dr Terry Roberts

9th IUPAC Symposium on Organometallic Chemistry Directed Towards Organic Synthesis, Göttingen, Germany, 20–25 July 1997

IUPAC SPONSORED

The most relevant topics at OMCOS 9 are:

- Catalytic transformations of organic molecules;
- Catalyst engineering;
- C–C and C–X bond forming processes mediated by metals;
- Creation of new materials using organometallics;
- Asymmetric synthesis applying organometallics and metal catalysis;
- Bond activation by metal complexes;
- Oligometal catalysis;
- Mechanistic and structural aspects of organometallic transformations;
- Oligo- and polymerizations under metal catalysis.

The symposium format includes the Springer Award Lecture, five plenary lectures and 19 invited lectures. In addition, there will be 19 short lectures. All attendees of OMCOS 9 are welcome to present a communication in poster form. The deadline for submission of abstracts is 1 June 1997. If oral presentation is not applied for, abstracts may be submitted until 1 July 1997. There will also be two to three separate poster sessions to provide opportunities for all to have scientific discussions.

The registration fee is DM 540 before 13 June 1997, DM 640 after 13 June 1997, for active participants, and DM 140 before 13 June 1997 and DM 170 after 13 June 1997, for students. Personal members of IUPAC are entitled to a 10% discount. A one-day ticket is also available at DM 260.

For further information on submission of a paper, please contact: Prof. Dr Armin de Meijere, Institut für Organische Chemie, Georg-August-Universität Göttingen, Tammannstr. 2, D-37077 Göttingen, Germany. Tel.: +49 (0)551 39 3232. Fax: +49 (0)551 39 9475. E-mail: ucoc@uni-goettingen.de

For further information on registration, please contact: Gesellschaft Deutsche Chemiker, Abteilung Tagungen, PO Box 90 04 40, D-60444 Frankfurt am Main, Germany. Fax: +49 (0)69 7917 475.

IAP97: Interfaces Against Pollution, Wageningen, the Netherlands, 10–13 August 1997

IUPAC SPONSORED

The general objective of IAP97 is to highlight interfacial (including catalytic) and colloidal aspects of environmental pollution and of technologies to monitor, remediate, reduce, abate and prevent pollution. Emphasis will be given to aquatic and soil systems. The idea of the conference was initiated by one of the subcommittees of the IUPAC Commission on Colloid and Surface Chemistry including Catalysis.

Topics include:

- Fundamental colloidal and interfacial aspects of monitoring, remediation and prevention;
- Colloid and interface science of particles and contaminants in the environment;
- Remediation and prevention;
- Environmental catalysis and bioremediation.

The conference fee is NLG 500 if paid before 31 May 1997; thereafter NLG 600. The fee covers coffee, tea, lunches and dinners (including the conference dinner) from Sunday until Wednesday.

For further information, please contact: the Conference Secretariat IAP97, PO Box 8038, 6700 EK Wageningen, the Netherlands. Tel.: +31 317 482279. Fax: +31 317 483777. E-mail: iap97@fenk.wau.nl.

Information about this conference is also available on the Internet on the IAP97 Home Page at http://ftp.fenk.wau.nl/iap.html

13th International Symposium on Plasma Chemistry, Beijing, China, 18–22 August 1997

IUPAC SPONSORED

The International Symposium on Plasma Chemistry (ISPC) is the main biennial international plasma chemistry symposium, encompassing the whole area of plasma chemistry, including near-equilibrium thermal plasmas and non-equilibrium plasmas. Topics will range from the basic physics and chemistry of plasmas to industrial processes and equipment. The symposium aims to facilitate the exchange of information and ideas between basic/applied researchers and practitioners of plasma processing technology. As is the tradition, the symposium will be preceded by a two-and-a-half day summer school on plasma chemistry. An industrial ex-

hibition of equipment and technology will be held concurrently with the symposium.

The symposium will consist of plenary lectures, parallel oral sessions of invited and contributed papers, poster sessions, and the colloquium on industrial applications of plasma chemistry.

The summer school will be held on 14–16 August 1997.

The symposium registration fee is USD 350 before 15 June 1997 and USD 400 after 15 June 1997; USD 175 before 15 June 1997 and USD 200 after 15 June 1997 for students. The registration fee includes attendance at sessions, proceedings, tea breaks, four lunches, welcome party and evening performance.

For further information, and details of fees for the summer school and exhibition, please contact: Mr. He Lin, Chinese Society of Theoretical and Applied Mechanics, No. 15 Zhong-guan-cun Rd, Beijing 100080, China. Fax: (86 10) 6255 9588 or (86 10) 6256 1284. E-mail: cstam@sun.ihep.ac.cn

12th Bratislava International IUPAC Conference on Polymers: Modified Polyolefins for Advanced Polymeric Materials, Bratislava, Slovak Republic, 25–28 August 1997

IUPAC
SPONSORED

The aim of the conference, organized by the Polymer Institute of the Slovak Academy of Sciences, is to bring together scientists from academia and industry to stimulate the exchange of ideas on recent advances in chemistry and physics of modified polyolefins. The programme will consist of main lectures, contributed lectures and posters devoted to the development of the methods of preparation and to the investigation of properties and morphology of modified polyolefins and /or multicomponent systems containing polyolefins.

The main topics are:

- Functionalization, grafting, crosslinking and reactive processing of polyolefins;
- Preparation and properties of polyolefin blends and composites;
- Special additives for polyolefins to increase their utility properties as well as to improve the processing into plastics products, films and fibres;
- New molecular structures in olefin homo- and copolymers.

The registration fee is CHF 390 (before 20 June 1997), CHF 430 after 20 June 1997; the IUPAC affiliated member fee is CHF 340 (before 20 June) and CHF 380 after 20 June; the fee for students is CHF 200 before 20 June and CHF 240 after 20 June. Fees include the conference proceedings, admission to all scientific sessions, refreshments, informal four lunches during the conference and the concert of the ensemble *Musa Ludens.*

For further information, please contact: Dr. Eberhard Borsig, Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, 842 36 Bratislava, Slovak Republic. Tel.: +42 1 7 378 2198. Fax: Savpolymer Bratislava 42 1 7 375923. E-mail: upolebor@savba.sk

7th International Symposium on Macromolecule–Metal Complexes, Leeuwenhorst Congres Centrum, Noordwijkerhout, the Netherlands, 6–10 October 1997

IUPAC
SPONSORED

The symposium will focus on the role of metal ions, complexes and clusters in macromolecular systems. The polymeric materials can be either natural, or synthetic organic, or synthetic inorganic. During recent years the scope of this field has widened significantly into the directions of supramolecular organic and inorganic chemistry. New insights have been developed into the role of the macromolecule on material properties such as catalysis, non-linear optics and electron transfer. Also many new synthetic methods have been developed, while the possibilities for characterization of such polymers have grown tremendously. The goal of the symposium is to bring together polymer chemists and technologists, synthetic chemists, coordination chemists and analytical/physical chemists. It is hoped that such a mix of investigators will lead to lively discussions and important cross-fertilization between fields.

The symposium will feature keynote and invited lectures, oral presentations and poster contributions.

The registration fee is NLG 900 (before 30 June 1997), NLG 1100 (after 30 June 1997). The registration fee includes coffee/tea and all lunches for the duration of the symposium, registration and one copy of the book of abstracts.

Information regarding the symposium will be updated periodically on the World Wide Web. Please contact http://wwwchem.leidenuniv.nl

For further information, please contact: Mrs. Y. Snellenberg, Symposium Secretary MMC-7, Leiden Institute of Chemistry, PO Box 9502, 2300 RA Leiden, the Netherlands. Tel.: +31 71 5274459. Fax: +31 71 5274451. E-mail: snellenb@chem.leidenuniv.nl

IUPAC International Conference on Biodiversity and Bioresources: Conservation and Utilization, Phuket, Thailand, 23–27 November 1997

IUPAC
SPONSORED

This international conference is organized by the National Center for Genetic Engineering and Biotechnology, the National Science and Technology Development Agency, under the auspices of IUPAC, and co-organized by the Chemical Society of Thailand.

The issues of biodiversity and bioresources affect a wide segment of the scientific world. The purpose of the conference is to stage a central event for the research community by presenting outstanding relevant developments in several areas and bringing together scientists from many disciplines from all over the world to discuss and exchange ideas on how biology, chemistry, biotechnology and other related fields might further enhance the conservation and utilization of bioresources.

The scientific programme includes a special keynote lecture, by Prof. Dr HRH Princess Chulabhorn Mahidol, plenary lectures and invited lectures, and mini symposia. In addition, ample time will be provided for poster presentations which will allow many participants to present their results to a wide international audience. Various social functions before, during and after the conference will be arranged for participants and accompanying persons.

The registration fee is USD 400 until 22 August 1997, and USD 500 after 22 August 1997, for participants, USD 360 until 22 August 1997, and USD 460, after 22 August 1997, for IUPAC affiliate members, and USD 200 until 22 August 1997, and USD 300, after 22 August 1997, for young scientists and students. The fees include registration, book of abstracts and final programme, formal reception on 23 November 1997, Poster-Thai cuisine cocktail and soft drinks on the evening of 25 November 1997, morning and afternoon coffee during 24–27 November 1997, lunches during 24–27 November 1997 and farewell dinner on 27 November 1997.

For further information, please contact: Prof. Dr. Sakarindr Bhumiratana, IUPAC Biodiversity Conference, National Center for Genetic Engineering and Biotechnology (BIOTEC), National Science and Technology Development Agency (NSTDA) Building, 73/1 Rama VI Road, Bangkok 10400, Thailand. Tel.: (662) 6448150-4 ext 505, 532, 534. Fax: (662) 6448107-8. E-mail: IUPACconf@biotec.or.th. Information and updates are also available on the Internet at http://www.biotec.or.th/Diary/IUPAC/IUPAC.htm

12th International Conference on Organic Synthesis, Venice, Italy, 28 June–2 July 1998

IUPAC
SPONSORED

This conference will emphasize all important aspects of the creative science of modern organic synthesis. The programme will include plenary lectures, section lectures, oral scientific contributions and poster presentations.

Topics to be highlighted include:

- New synthetic methods;
- Stereoselective synthesis;
- Metal-mediated synthesis;
- Target oriented synthesis.

In addition, there will be a mini symposium on combinatorial chemistry in drug discovery.

The following prominent scientists have agreed to present plenary lectures: S.G. Davies (UK), S. E. Denmark (USA), D. Kahne (USA), J. Mulzer (Germany), D.N. Reinhoudt (the Netherlands), P. Sinaÿ (France), A.B. Smith, III (USA), A. Togni (Switzerland), H. Yamamoto (Japan) and L. Paquette (USA).

An attractive social programme including the welcome cocktail on Sunday 28 June, a concert and the social dinner will be organized for participants and their accompanying persons.

A second circular will be available in September 1997, and will contain information on call for papers, registration, hotel accommodation and social programme. This second circular may be obtained from:

The Organizing Secretariat, ICOS-12, Depha Congress srl, Viale Majno 21, 20122 Milano, Italy. Tel.: +39 2 76 00 81 90. Fax: +39 2 78 24 00. E-mail: Dephadue@mbox.vol.it

7th International Chemistry Conference in Africa and 34th Convention of the South African Chemical Institute, Durban, South Africa, 6–10 July 1998

IUPAC SPONSORED

The scientific programme will cover all aspects of chemistry and will include several plenary and invited lectures, oral communications and poster presentations. Pre-conference workshops on various topical aspects of analytical chemistry are being planned for the Saturday prior to the start of the conference. Potential participants are invited to let the conference organizer know of particular interests. Ample space will be provided for the exhibition of scientific equipment, books and other related materials. Social activities such as a welcoming reception, banquet, excursions, accompanying persons programme and other events are also being planned.

A second circular and call for abstracts is planned for 30 August 1997.

Enquiries and correspondence should be sent to: The Secretary, 7th ICCA & 34th SACI Convention, Department of Chemistry & Applied Chemistry, University of Natal, Durban 4041, South Africa. Tel.: +27 31 260 3090. Fax: +27 31 260 3091. E-mail: 7icca@che.und.ac.za

9th International Symposium on Novel Aromatic Compounds (ISNA-9), Hong Kong, 2–7 August 1998

IUPAC SPONSORED

The main objective of this symposium series is to generate channels for the interflow of innovative ideas among practising chemists world-wide. ISNA-9 will provide an international forum for presentation and discussion, by both professionals and students alike, of new findings in all aspects of chemistry concerning molecules with conjugated π-systems.

Topics to be discussed will include:

- Novel aromatic and anti-aromatic compounds;
- New π-topologies;
- Electronic materials containing π-systems;
- Molecular recognition and self-organization;
- Functionalized aromatics as synthetic building blocks and catalysts;
- Carbon allotropes;
- Theory of π-systems.

The symposium scientific programme will consist of:

- The First Nozoe Memorial Lecture and 14 plenary lectures;
- 23 invited lectures;
- Poster presentations.

The registration fee is USD 390 for active participants, and USD 130 for *bona fide* student participants.

For further information, please contact: Prof. Henry N. C. Wong, Department of Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong. Tel.: +852 2609 6344. Fax: +852 2603 5057. E-mail: hncwong@cuhk.edu.hk

XIX International Carbohydrate Symposium, San Diego, California, USA, 9–14 August 1998

IUPAC SPONSORED

The scientific programme will cover:

- Structure and analysis: primary, secondary and higher order structure, conformational analysis, spectroscopic and instrumental analysis;
- Synthesis: chemical and enzymatic synthetic methods, synthesis of carbohydrates, nucleosides, nucleotides, antibiotics involving carbohydrate moieties, carbohydrates as chiral synthons;
- Biological and medicinal chemistry: biological function, metabolic role, pharmaceutical and therapeutic implications;
- Biotechnology, ecology and industry: commercial applications of carbohydrates, methods of production, novel or unique industrial and ecological developments

The symposium will include plenary lectures, invited lectures and contributed papers. Approximately 100 of the contributed papers will be selected for oral presentation; the remainder will be presented in poster sessions.

For further information, please contact: ICS 98 Symposium Secretariat, Department of Chemistry, 516 Physical Sciences 1, University of California, Irvine, CA 92697-2025, USA. Tel.: +1 714 824 8976. Fax: +1 714 824 1372. E-mail: ics98@uci.edu. Information is also available on the World Wide Web at http://www.ics98.uci.edu

21st IUPAC International Symposium on the Chemistry of Natural Products (ISCNP-21), Beijing, China, 11–16 October 1998

IUPAC SPONSORED

The Chinese Chemical Society invites submission of abstracts for oral or poster sessions at this symposium, which will include plenary and invited lectures, poster and short oral presentations.

The fields to be covered can be roughly defined as:

- Isolation, structure and elucidation including modification of natural products, and the structure-activity relationship;
- Synthesis of natural products and related compounds, including synthetic reactions, synthetic methodology and especially stereoselective synthesis;
- New methodology and techniques for isolation and structure determination, especially modern NMR, MS techniques and computer aided structure elucidation;
- Biosynthesis, biomimetic syntheis and biogenesis of natural products;
- The chemistry and biological activity of marine natural products;

An exhibition of books, instruments, chemicals and information of interest to chemists will be held during the symposium.

A post-symposium on synthesis of natural products will be held in Shanghai on 18–19 October 1998.

For further information on ISCNP, please contact: Prof. Xibai Qiu, Secretariat of ISCNP-21, c/o Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: 86 10 62568157, 62564020; Fax: 86 10 62568157; E-mail: qiuxb@infoc3.icas.ac.cn

For information on the post-symposium in Shanghai, please contact: Prof.Guoqing Lin, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 354 Fenglin Road, Shanghai 200032, China. Tel.: 86 21 64163300. Fax: 86 21 64166128, 64166263. E-mail: lingq@pub.sioc.ac.cn

Conference Calendar

1997

High temperature materials chemistry

19–23 May

9th International Conference on High Temperature Materials Chemistry (HTMC IX). Pennsylvania State University, PA, USA.

Judy Hall, Conference Planner, Pennsylvania State University, 225 Penn State Conference Center, University Park, PA 16802–7002. Tel.: +1 (814) 8635130. E-mail: conferenceinfo1@cde.psu.edu, WWW site: URL:http://www.cde.psu.edu/C&I/htmc/

Bioorganic chemistry

1–6 June

4th International Symposium on Bioorganic Chemistry. Biarritz, France.

Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45–4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Molecular architecture for degradable polymers

10–14 June

International Symposium on Molecular Architecture for Degradable Polymers: Molecular Design of Polymeric Materials of Tomorrow. Stockholm, Sweden.

Prof. Ann-Christine Albertsson, Department of Polymer Technology, KTH, Royal Institute of Technology, S-100 44 Stockholm, Sweden. Tel.: +46 (8) 7908274. Fax: +46 (8) 100775.

Electrochemical processes at liquid interfaces and membranes

15–20 June

30th Heyrovsky Conference on Electrochemical Processes at Liquid Interfaces and Membranes, Moravia, Czech Republic.

Prof. Z. Samec, J. Heyrovsky Institute of Physical Chemistry, Dolejskova 3, 182 23 Prague 8, Czech Republic.

Polymer synthesis

16–20 June

International Symposium on New Approaches in Polymer Synthesis and Macromolecular Formation. St. Petersburg, Russia.

Mrs. Irina Kovalenko (Symposium Coordinator), Institute of Macromolecular Compounds, Bolshoy pr. 31, 199004 St. Petersburg, Russia. Tel.: +7 (812) 2131070. Fax: +7 (812) 2186869. E-mail: imc@macro.spb.su

Ionic polymerization

7–11 July

International Symposium on Ionic Polymerization. Paris, France.

Symposium Secretariat, Chantal Iannarelli, Congrès Scientifiques

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy.

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

Services, 2 Rue des Villarmains, F-92210 Saint-Cloud, France. Tel.: +33 (1) 47 71 90 04. Fax: +33 (1) 47 71 90 05.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic. Tel.: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Vacuum microbalance techniques

16–18 July
27th International Conference on Vacuum Microbalance Techniques. Lublin, Poland.
Dr P. Staszczuk, Department of Physical Chemistry, Faculty of Chemistry, Marie Curie-Sklodowska University, M. Curie-Sklodowska Sq. 3, 20–031 Lublin, Poland. Tel.: +48 (81) 5375646/+48 (81) 5375784. Fax: +48 (81) 5333348. E-mail: piotr@hermes.umcs.lublin.pl/ rdobrow@hermes.umcs.lublin.pl

Organometallic chemistry

20–25 July
9th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis. Göttingen, Germany.
Prof. A. de Meijere, Chairman OMCOS 9, Institut für Organische Chemie, Georg-August-Universität Göttingen, Tammannstrasse 2, D-37077 Göttingen, Germany. Tel.: +49 (551) 39 32 32. Fax: +49 (551) 39 9475. E-mail: ucoc@uni-goettingen.de

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules, Surface and Interfacial Phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic. Tel.: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Bioinorganic chemistry

27 July-1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan. Tel.: +81 (3) 38122111 ext. 7261. Fax: +81 (3) 58006945

Medicinal chemistry

29 July–1 August
AIMECS'97: AFMC International Medicinal Chemistry Symposium. Seoul, Korea.
Dr. H. Park, Secretary General, AIMECS 97, c/o The Korean Chemical Society, #703, The Korean Science & Technology Center, 635-4, Yeogsam-Dong, Kangnam-Gu, Seoul 135-703, Korea. Tel.: +82 (2) 34534019. Fax: +82 (2) 5696673. E-mail: hpark@kistmail.kist.re.kr

Interfaces against pollution

10–13 August
International Conference on Interfaces Against Pollution. Wageningen, Netherlands.
IAP97, P.O. Box 8038, 6700 EK Wageningen, Netherlands. Tel.: +31 (317) 482279. Fax: +31 (317) 483777. E-mail: iap97@fenk.wau.nl

Plasma chemistry

18–22 August
13th International Symposium on Plasma Chemistry. Beijing, China.
Dr Lin He, Chinese Society of Theoretical & Applied Mechanics, 15 Zhong Guan Cun Road, Beijing 100080, China.

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
AKM Congress Service, PO Box 37, CH-1218 Le Grand-Saconnex/GE, Switzerland. Tel.: +41 (22) 7611661. Fax: +41 (22) 7611662.

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion.

Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile.
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (2) 6811644. Fax: +56 (2) 6812108. E-mail: jcostama@lauca.usach.cl

Polymers

25–28 August
12th Bratislava Conference on Polymers: Modified Polyolefins for Advanced Polymeric Materials. Bratislava, Slovak Republic.
12th Bratislava International Conference on Polymers, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, 842 36 Bratislava, Slovak Republic. Tel.: +42 1 (7) 3782198. Fax: +42 1 (7) 375923. E-mail: upolebor@savba.sk

Solution chemistry

26–31 August
24th International Conference on Solution Chemistry, Centre Omnisport, Vichy, France.
Prof. P. Turq, Laboratoire d'Electrochimie, Université Pierre & Marie Curie, Case courier 51, 4 place Jussieu, 75252 Paris Cedex 05, France

Electron transfer processes

3–7 September
International Symposium on Electron Transfer Processes and Reactive Intermediates in Macromolecular and Organic Chemistry. Zabre, Poland.
Prof. Z.J. Jedlinski, Institute of Polymer Chemistry, Polish Academy of Sciences, ul. Marii Curie Sklodowskiej 34, 41–800 Zabrze, Poland. Tel.: +48 (32) 1716077. Fax: +48 (32) 1712969. E-mail: polymer@usctoux1.cto.us.edu.pl

Colloquium spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997. Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel.: +61 (3) 98193700. Fax: +61 (3) 98195978.

Emulsions

23–26 September
2nd World Congress on Emulsions: Industrial Applications of Emulsions. Bordeaux, France.
Mr A. Le Coroller, Directeur-Général, CME, 50 place Marcel Pagnol, 92100 Boulogne-Billancourt, France. Tel.: +33 (1) 47617689. Fax: +33 (1) 47617465.

Macromolecule–metal complexes

6–10 October
7th International Symposium on Macromolecule-Metal Complexes (MMC-7). Noorwijkerhout, Netherlands.
Prof. J. Reedijk, Leiden Institute of Chemistry, PO Box 9502, 2300 RA Leiden, Netherlands. Tel.: +31 (71) 5274459. Fax: +31 (71) 5274451. E-mail: reedijk@rulgca.leidenuniv.nl

Biodiversity and bioresources

23–27 November
International Conference on Biodiversity and Bioresources—Conservation and Utilization. Phuket, Thailand.
IUPAC Biodiversity Conference, National Center for Genetic Engineering and Biotechnology, National Science and Technology Development Agency Building, 73/1 Rama VI Road, Bangkok 10400, Thailand. Tel.: +66 (2) 6448150–4, ext. 505, 532, 534. Fax: +66 (2) 6448107–8. E-mail: iupacconf@biotec.or.th

1998

Polymer sciences and technology

5–10 January
International Symposium on Advances of Polymer Sciences and Technology. Madras, India.
Dr K.S.V. Srinivasan, Deputy Director & Head, Polymer Division, Central Leather Institute, Council of Scientific & Industrial Research, Adyer, Madras - 600 020, India.

Calorimetry and chemical thermodynamics

5–9 April
International Conference on Calorimetry and Chemical Thermodynamics. Campinas, Brazil.
Prof. C. Airoldi, Instituto de Química, UNICAMP - CP 6154, Universidade Estradul de Campinas, 13081-970 Campinas sp, Brazil.

Trace element speciation

4–7 May
1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences. Neuherberg, Munich, Germany.
First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, Germany. Tel.: +49 (89) 31873030 (2669). Fax: +49 (89) 31873362.

Degradation processes in the environment

24–28 May
International Conference on Degradation Processes in the Environment. Dubrovnik, Croatia.
Dr A. Sabljic, Institute Boskovic, PO Box 1016, HR-10011 Zagreb, Croatia.

Organic synthesis

28 June–2 July
12th International Conference on Organic Synthesis. Venice, Italy.
Depha Congress SRL, Viale Majno 21, 20122 Milano, Italy. Tel.: +39 (2) 76008190. Fax: +39 (2) 782400. E-mail: dephadue@mbox.vol.it

Chemistry in Africa

6–10 July
7th International Chemistry Conference in Africa (7th ICCA). Durban, South Africa.
The Secretary, 7th ICC & 34th SACI Convention, Department of Chemistry & Applied Chemistry, University of Natal, Durban 4041, South Africa. Tel.: +27 (31) 2603090. Fax: +27 (31) 2603091. E-mail: 7icca@che.und.ac.za

Macromolecules

20–23 July
18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.
P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, CZ-162 06 Prague 6, Czech Republic. Tel.: +420 (2) 360341. Fax: +420 (2) 367981. E-mail: sympo@imc.cas.cz

Chemical thermodynamics

26 July-1 August
15th International Conference on Chemical Thermodynamics. Porto, Portugal.
Prof. M.A.V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal.

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (171) 4378656. Fax +44 (171) 7341227.

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chemistry International* 1992, **14**, 203.

Solubility phenomena

5–8 August
8th International Symposium on Solubility Phenomena. Niigata, Japan.
Prof. H. Akaiwa, Faculty of Engineering, Gunma University, Kiryu 376, Japan.

Physical organic chemistry

16–21 August
14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.
Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento di Química, 88040–900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy. Tel.: +39 (55) 2757549. Fax: +39 (55) 2757555.

Natural products

11–16 October
21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.
Prof. Xibai Qiu, Secretariat of ISCNP-21, c/o Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: +86 (10) 62568157 or 62564020. Fax: +86 (10) 62568157. E-mail: qiuxb@infoc3.icas.ac.cn

2000

Macromolecules

9–14 July
MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.
Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90-363 Lodz, Poland. Tel.: +48 (42) 819815. Fax: +48 (42) 847126.

Biotechnology

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.

Stop press

The move of the Secretariat Office from Oxford to Research Triangle Park (RTP), North Carolina, is underway, with a transition period that will last from May through September. During this time much of the Secretariat's work will continue to be done in Oxford, and all correspondence should be directed to that office. Material will be forwarded to the new Executive Director, Dr John Jost, as needed. Although Dr Mo Williams retired as of the end of April, he has agreed to assist Dr Jost in a consulting capacity for the next few months. This will greatly facilitate the smooth transfer of operations.

The staff at RTP is currently only Dr Jost. He will be adding staff over the next few months as more functions are moved from Oxford to RTP. A number of key items regarding the transition are summarized in the following list:

- All expense claims will continue to be handled by Mrs Erica Sheppard until October.
- All preparation and support work for the General Assembly in Geneva will be handled from Oxford.
- All change of address notices and information regarding new members of Commissions and other IUPAC bodies should continue to be sent to Oxford until October.
- Mr Mervyn Richardson, Acting Scientific Publications Secretary, has agreed to continue working on *Pure and Applied Chemistry* through the last issue of 1997 and to complete the subject index.
- Dr Mo Williams has agreed to coordinate the work on *Chemistry International* through the last issue of 1997.
- All work relating to Symposia, Commission Reports and Books which will be published in 1998 or later will be done at RTP.
- In October the Oxford office will be occupied in shipping files to RTP and to the Chemical Heritage Foundation in Philadelphia and in disposal of furniture and equipment.

The address of the office in RTP is:
IUPAC Secretariat
PO Box 13757
Research Triangle Park, NC 27709-3757, USA.

The telephone number of the RTP office is 919 485 8700, the Fax is 919 485 8706 and Dr Jost's E-mail is johnwjost@compuserve.com. Please feel free to call, write or send an e-mail if you have any questions.

Blackwell Science

Osney Mead,
Oxford OX2 0EL,
UK

Telephone
(01865) 206206

Fax
(01865) 206096

INTERNATIONAL JOURNAL OF FOOD SCIENCE AND TECHNOLOGY

Published for the Institute of Food Science and Technology (UK) by Blackwell Science Ltd

Editor: **Dr D G Land**, *Norwich*

The scope of this authoritative journal covers a wide field, ranging from pure research in the various sciences associated with food to practical experiments designed to improve technical processes. While the main object is to provide a forum for papers describing the results of original research, review articles are also included. Manuscripts of original research or comprehensive reviews of specialized sections of food science or technology are welcomed. The editor maintains the high standards of selection and criticism to ensure that only those papers which make a significant contribution to the technology are published. The journal is covered by Current Contents, ASCA and Science Citation Index.

Subscription Information

International Journal of Food Science and Technology is published bimonthly. Subscription rates for 1997 are £235.00 (Europe), £258.00 (Overseas) and US$408.00 (North America).

Order Form

Please tick the appropriate box and return to Karen Edge at the address opposite:

☐ I would like to subscribe to *International Journal of Food Science & Technology*

☐ I wish to pay by cheque and enclose the sum of £_____ US$_____

☐ I wish to pay by Access/American Express/Barclaycard/Diners Card/VISA/Mastercard/JCB (delete as necessary). Please debit my credit card no.

Expiry date_____

with the sum of £____ US$____ Signature_____ Date_____

European Community VAT & Canadian GST

Subscribers in Europe must quote their VAT registration number or state that they are not VAT-registered. Subscribers in the following countries who are not VAT-registered must add VAT to the subscription price at the appropriate rate: Belgium (6% TVA/BTW); France (2.1% TVA); Germany (7% MwSt); Spain (4% IVA); The Netherlands (6% BTW).

All subscribers in Canada must add 7% to allow for GST.

VAT registration number_____ I am not registered for VAT ☐

☐ Please send me a specimen copy of *International Journal of Food Science and Technology*

Name_____

Address_____

_____

Blackwell Science

Osney Mead,
Oxford OX2 0EL,
UK

Telephone
(01865) 206206

Fax
(01865) 206096

Pure and Applied Chemistry

IUPAC

Official Journal of the International Union of Pure and Applied Chemistry

Since 1960 the Union has made available to chemists everywhere a very large amount of important material which it handles each year through its regular publication in Pure and Applied Chemistry. The objectives of the journal are:

- to publish the main invited lectures of symposia sponsored by IUPAC at which authoritative and up-to-date accounts of the subject of the symposium are presented by prominent scientists; the lecturers cover their own recent work and review the worldwide literature on the subject;
- to publish the recommendations of the Union's commissions on nomenclature, symbols and units;
- to publish technical reports on standardization, recommended procedures, collaborative studies, data compilations, etc.;
- to publish critically evaluated state-of-the-art commissioned review articles on important topics.

Subscription Information

Pure and Applied Chemistry is published monthly. Subscription rates for 1997 are for institutions are £672.00 (Europe), £736.00 (overseas) and US$1020.00 (USA & Canada). Individual subscription prices for 1997 are £82.00 (Europe), £82.00 (overseas) and US$115.00 (USA & Canada).

Order Form

Please tick the appropriate box and return to Karen Edge at the address opposite:

☐ Please enter my 1997 Institutional subscription to *Pure and Applied Chemistry*

☐ Please enter my 1997 Individual subscription to *Pure and Applied Chmistry*

☐ I wish to pay by cheque and enclose the sum of £_____ US$_____

☐ I wish to pay by Access/American Express/Diners Card/VISA/Mastercard/JCB

(delete as necessary)

Please debit my credit card no. | | | | | | | | | | | | | | | | |

Expiry date _____ with the sum of £_____ US$_____

Signature _____ Date _____

European Community VAT & Canadian GST

Subscribers in Europe must quote their VAT registration number or state that they are not VAT-registered. Subscribers in the following countries who are not VAT-registered must add VAT to the subscription price at the appropriate rate: Belgium (6% TVA/BTW); France (2.1% TVA); Germany (7% MwSt); Spain (4% IVA); The Netherlands (6% BTW).

All subscribers in Canada must add 7% to allow for GST.

☐ Please send me a specimen copy of *Pure and Applied Chemistry*

Name _____

Address _____

_____

http://www.blackwell-science.com

International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

President: A. E. FISCHLI (*Switzerland*)
Vice-President: J. JORTNER (*Israel*)

Secretary-General: E. D. BECKER (*USA*)
Treasurer: J. M. WARD (*UK*)

IUPAC Secretariat

Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK.
Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 38 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Neue Schweizerisches Chemische Gesellschaft **(Switzerland)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1997, Vol. 19, No. 3 (May)

65 News

70 Commission News

72 PAC Review

75 Recent Reports

79 New publications

82 Provisional Recommendations

83 Conference Report
Prof. Pieter Steyn and Dr Terry Roberts

86 Conferences

90 Conference Calendar

94 Stop Press

Information on this magazine can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Blackwell Science

0193-6484(199705)19:3:1-2

Printed in Great Britain by Alden, Oxford, Didcot & Northampton

ISSN 0193-6484

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

1997, Vol. 19, No. 4 (July)

b

Blackwell Science

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

ACTING EDITOR: Mike Ward
PRODUCTION EDITOR: Howard Waller

All correspondence to be addressed to The Editor, Chemistry International, IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK. Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk and http://chemistry.rsc.org/rsc/iupac.htm

Editorial Advisory Board

Chairman:	E. D. BECKER	*Secretary General*		
	E. BUNCEL	*CHEMRAWN Committee*		
	A. SMITH	*Committee on Chemistry and Industry*		
	D. H. M. BOWEN	*Committee on Printed and Electronic Publications*		
	I. M. MILLS	*Interdivisional Committee on Nomenclature and Symbols*		
	M. E. PESTANA	*Committee on Teaching of Chemistry*	(To be appointed)	*Division VII*
Acting Secretary:	J.W. JOST	*Executive Director*		
			G. SOMSEN	*Division I*
			G. J. LEIGH	*Division II*
			G. SAVELLI	*Division III*
			A. ABE	*Division IV*
			F. INGMAN	*Division V*
			T. R. ROBERTS	*Division VI*

Subscriptions

Six issues of *Chemistry International* will be published bimonthly in 1997. The 1997 subscription rate including postage is GBP 75.00 (UK and overseas except North America) or USD 116.00 (US and Canada). The individual subscription rate is GBP 29.00 (UK and overseas except North America) or USD 42.00 (US and Canada). Microfiche subscriptions are available simultaneously with the printed edition, and microfilm at the end of the subscription year. Subscription orders may be placed directly with IUPAC's official publisher, Blackwell Science Ltd, PO Box 88, Oxford, UK; E-mail: journals.cs@blacksci.co.uk. Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Advertising. Enquiries should be sent to the Advertising Manager, Blackwell Science Ltd, Osney Mead, Oxford OX2 0EL, UK. Telephone: +44 (0) 1865 206206, Telex 83355 Medbok G, Fax +44 (0)1865 721205.

Despatch. The news magazine is despatched within Europe by surface mail, to other continents by various forms of air-speeded delivery: to the US* by air freight for forwarding by periodicals post, to India by air freight for guaranteeed local delivery, and to all other countries by Accelerated Surface Post.

Reproduction of Articles

Unless there is a footnote to the contrary, reproduction or translation of articles in this issue is encouraged, provided that it is accompanied by a reference to the original in *Chemistry International.* The Blackwell Science logo is a trade mark of Blackwell Science Ltd registered at the United Kingdom Trade Marks Registry.
This journal is included in the ADONIS service, whereby copies of individual articles can be printed out from compact discs (CD-ROM) on demand.

*Periodicals postage paid at Rahway, NJ. Post Master, send address changes to *Chemistry International*, c/o Mercury Airfreight International Inc., 2323 Randolph Avenue, Avenel, NJ 07001, USA.

Front cover: The Sciences II Building of the University of Geneva which will host the 39th IUPAC General Assembly (see pages 96–104).

Secretary General's Column

Edwin D. Becker

During the last few months, the IUPAC Officers, Division Presidents, and others have spent a great deal of time considering the mission and structure of the Union in order to position IUPAC to best meet the challenges of the coming decade. As a prelude to the 39th General Assembly (see pages 96–104), I would like to give a summary of some of the major activities and actions.

Outside advice

As I indicated in a previous column (*Chem. Int.*, January 1997, pages 6–7), we held a meeting in London on 24 February, which brought together ten leaders in chemistry from eastern and western Europe. This meeting was a follow-up to one in North America (at the Belmont Conference Center). The London meeting was aimed at obtaining guidance on IUPAC's future roles in such areas as the objectives and priority areas of the Union; the service of chemistry to society, developing countries and the international community in general; the role of the Union in chemical education at all levels; international communication in the chemistry community; and the organization of IUPAC. The group provided 21 thoughtful recommendations on these and other topics. Many recommendations were reflected in later actions, as described below.

The third and final meeting in this series was held in Singapore on 21 June to sample opinion from a number of scientific leaders in the Asia/Pacific region. Recommendations will be available to the IUPAC Bureau for action at the General Assembly in Geneva.

Vice-President's Critical Assessment (VPCA)

Under our Bylaws, 'The Vice-President shall submit to the Bureau biennially a critical assessment of the programmes and projects of all IUPAC bodies'. Vice-President Jortner divided his 1997 Assessment into two major parts–Science Policy of the Union, and Structure and Function. In Part I, he commented on principles, general activities and future directions of the Union. In line with recommendations from the Belmont and London meetings, he proposed augmenting the general Objectives in the IUPAC Statutes with 13 Goals that would better define the mission and activities of IUPAC for the next few years. In Part II, he analyzed the current Divisional and Commission structure, and recommended specific changes to improve interdisciplinary activities and to close gaps in the Union's activities.

It is not possible here to give details of Prof. Jortner's VPCA, which runs to 34 pages. Copies have been distributed to Division Committees, Commission and Committee Officers and National Adhering Organizations and will be available at the General Assembly.

Organization and Management of IUPAC's Scientific Work

A special meeting of Division Presidents and Vice-Presidents in Frankfurt on 24 March focused on ways in which many of the recommendations in the VPCA can be implemented. The principal items discussed involve improved allocation of resources, possible modifications in the structure of Commissions and conduct of interdivisional activities. A major objective of virtually all participants was an increase in flexibility for Division Committees.

Building on the ideas expressed at this meeting and on historical efforts to bring about needed changes in the structure and operation of the Union, I presented to the Executive Committee (EC) at its meeting in Jerusalem on 6–7 April 1997 a paper that advocated moving much of our scientific work to a project-driven structure, with primarily time-limited Commissions selected to carry out well-defined projects in a specific period of time. Under this approach, Divisions would regard the entire worldwide chemical community as the resource both for ideas and for volunteers to carry out projects. Just how to generate such ideas, develop projects and seek out people able and willing to work on the projects is, of course, the key to success or failure. I am con-

vinced that ideas for useful work usually originate in a 'bottoms-up' manner, not as directed from 'top-down'. In fact, the establishment of the pool of Titular Members was to permit the undertaking of such 'top-down' projects generated outside the mainstream of Commission activity, but after several years there are very few such projects. If we implement the type of structure envisioned here, but without a good mechanism to identify and develop projects—and to secure the services of experts on the Commissions—we will destroy the valuable work that is now being done by Commissions. A great deal of thought and planning is needed to ensure that IUPAC can develop the processes to do this without the large cadre of long-term members of Commissions.

In this space I cannot begin to list the many advantages and possible pitfalls that I see in modifying our organization and procedures, and I am sure there are many others that I have not envisioned. The EC discussed this proposal in detail and decided to adopt the concept, but with the recognition that many details must be examined before it can be implemented. The EC also endorsed in principle the recommendations in the VPCA to establish clear Goals for IUPAC but, again, recognized that further thought and discussion are needed to refine the Goals. The EC concluded that a broad-based committee would be needed to develop the necessary strategic thrusts and to consider their implementation in terms of the structure and guidelines for scientific activity. The EC therefore authorized the formation of a Strategy Development and Implementation Committee (SDIC), to report back to the EC in April 1998. From the findings and recommendations of the SDIC, the EC expects to formulate specific proposals for approval by the Bureau in September 1998 and for necessary action by Council in 1999.

The SDIC, under the chairmanship of the President-Elect, includes representation from the Divisions, the Bureau, the Officers and the chemistry community at large. The Committee held its initial meeting on 24 June, so that some preliminary views might be reported to the Bureau and Council in Geneva.

39th IUPAC General Assembly

IUPAC General Assemblies are held in odd-numbered years. This year, the 39th General Assembly, will take place at the University of Geneva, Switzerland, 23–30 August. The General Assembly follows immediately after the 36th IUPAC Congress to allow participants to attend both events.

Prof. Jacques Weber, Chairman of the local Organizing Committee in Switzerland, writes:

The IUPAC General Assembly has little in common with a scientific conference or congress. It is indeed not open for general participation but restricted to Members of IUPAC Bodies that meet on this occasion. This is the case for practically all the IUPAC Committees and Commissions, which meet during the first half of the General Assembly, followed by the meeting of the IUPAC Council (see page 97).

The average attendance at these General Assemblies is 600–700 participants, the major problem being that the meeting of all the IUPAC Bodies may require the simultaneous use of up to 50 seminar rooms of various capacities (typically 10–30 seats) on the same site! In view of this constraint, it rapidly appeared that the University of Geneva was an ideal location for the General Assembly, especially as the modern Uni Mail Building offers very good facilities of that sort. Both Sciences II and Uni Mail Buildings will therefore share the venue of the General Assembly, with 26 meeting rooms reserved in the first facility and 24 in the second. These buildings lie quite close to one another, at a 10-minute walking distance, which should not be a problem for the delegates. In addition, both buildings are modern with large open spaces, ample photocopying capacity, and availability of computer rooms and cafeterias.

The whole scientific programme of the General As-

Prof. Jaques Weber

sembly is prepared by IUPAC itself, the local organizers being in charge of the accommodation, administrative secretariat, meeting rooms, social programme and financing. Indeed, as far as the latter point is concerned, the rule is that the host country finances the General Assembly, IUPAC making a financial contribution towards the subsistence and travel expenses of its Titular Members.

The first IUPAC General Assembly was organized in Rome in 1920; the most recent took place in Guildford, UK, in 1995. The IUPAC General Assemblies have been held three times before in Switzerland (Lucerne/Zürich, 1936; Zürich, 1955; Davos, 1979). A local Organizing Committee for the IUPAC Congress and General Assembly was set up by the New Swiss Chemical Society (NSCS) in March 1995. This followed a visit to Geneva of several members of the Oxford IUPAC Secretariat who found adequate both the venues chosen for the events and the conditions of accommodation.

In May 1995, the decision was made by IUPAC to hold the 39th General Assembly in Geneva. The decision was made in July 1995 also to hold the 36th IUPAC Congress in Geneva. The organizers expect that the competence and enthusiasm of the volunteers (students and staff of the Section of Chemistry of the University of Geneva) will lead to a successful 39th IUPAC General Assembly.

Adapted from *Chimia* 1996, **50**(6).

39th IUPAC Council Meeting

University of Geneva, Switzerland
29–30 August 1997

Election of Officers and Bureau Members

According to Statute 5.401, Council must elect:
(i) Officers of the Union
(ii) Elected Members of the Bureau

Nominations for the various positions that fall vacant at the end of 1997 must be received by the Secretary General at the IUPAC Secretariat before 29 June 1997, i.e. two months before the start of the Council meeting (Bylaw 2.221). The situation for each position (as this issue went to press on 20 June) is set out on pages 98–104:

President
Prof. J. Jortner (Israel), Vice-President and President-Elect, becomes President on 1 January 1998 (Statute 4.2).

Vice-President—Vacancy
The Vice-President to be elected at the 39th Council Meeting will be President-Elect, and will become President on 1 January 2000.

Council Agenda

1 Introductory Remarks and Finalization of Agenda
2 Approval of Minutes of 38th Council Meeting and Matters Arising
3 Ratification of Decisions Taken by Bureau and Executive Committee since 38th General Assembly
4 Announcement of Nominations for Union Officers and Bureau Members
5 Announcement of Time of Elections
6 Statutory Report of President on State of Union
7 Report of Secretary General
8 Biennial Report of Treasurer/Report of Finance Committee and Accounts for 1995–6/Appointment of Auditors for 1997–8
9 Reports of Division Presidents (10 minutes each)
10 Report of Committee on Printed and Electronic Publications (10 minutes only)
11 Report of CHEMRAWN Committee (10 minutes only)
12 Report of Committee on Chemistry and Industry (10 minutes only)
13 Report of Committee on Teaching of Chemistry (10 minutes only)
14 Report on and Review of Affiliate Membership Programme
15 Proposed Changes to Statutes and Bylaws
16 Continuation/Dissolution of Existing IUPAC Bodies, Proposals for New and Reconstituted Bodies/Terms of Reference
17 Proposals Formally Received from National Adhering Organizations
18 Ratification of Dates and Places of 40th General Assembly and 37th Congress (1999)
19 Budget Proposal and National Subscriptions for 1998–9
20 Election of Union Officers and Bureau Members and Approval of Elected Officers of Divisions
21 Provisional Places of 41st General Assembly and 38th Congress (2001)
22 Applications for Membership of IUPAC
23 Applications for Associated Organization Status of IUPAC and Review of Existing Associated Organizations
24 Adoption of Recommendations on Nomenclature and Symbols
25 Important Matters Discussed by Bureau at 39th General Assembly Not Covered by Items on Council Agenda
26 Any Other Business (discussion only)

Nominations for Vice-President received (as at 20 June 1997) are: Prof. P.S. Steyn (South Africa) and Dr A. Hayes (UK).

Prof. Pieter S. Steyn (South Africa)

Pieter Streicher Steyn was born on 5 January 1940 in Vryburg, Cape Province, Republic of South Africa. He is married with three children.

Education and Career: Prof. Steyn studied at the University of Stellenbosch, Stellenbosch: BSc, 1959; BSc (Hons), 1962; MSc (*cum laude*), 1963, and then at the University of South Africa: PhD, 1966. In 1967 he was awarded a Post-doctoral Fellowship at the School of Pharmacy of the University of Wisconsin, Madison, USA. He was appointed to the National Chemical Research Laboratory, CSIR in 1964 where he became Head of the Division of Organic Chemistry in 1983. From 1986 to 1987 he was Chief Director of the National Food Research Institute, CSIR, and from 1987 to 1992 he was Director of the Division of Food Science and Technology, CSIR. In December 1992, Prof. Steyn was appointed the first CSIR Fellow, this being the highest career position in science within the CSIR. In October 1993, he was appointed Head of the SASOL Centre for Chemistry, SASOL Professor of Chemistry and Director of the SASOL Centre of Separation Technology at the Potchefstroom University for Christian Higher Education.

Research Interests: Prof. Steyn's research career has been devoted to the isolation, analysis, structure elucidation, synthesis and biosynthesis of mycotoxins and, to some extent, other toxic and medicinal substances from plants. This research has been undertaken with numerous groups within South Africa and with research groups in Australia, Europe, Japan, New Zealand and the USA. Prof. Steyn has authored or co-authored 153 scientific papers and 20 reviews.

Offices and Assignments: These include: Elected one of 54 Founder Members of the Academy of Science of South Africa (1994-present); Vice-President of the South African Joint Council of Scientific Societies (1985–86); President of the South African Joint Council of Scientific Societies (1986–87) and President of the International Association for Cereal Science and Technology, Vienna (1992–94).

Since 1967, Prof. Steyn has given lectures at the Conventions of the South African Chemical Institute, at the Specialist Conference on Organic Chemistry, and been invited to speak at numerous international meetings.

IUPAC Activities: Member of the South African National Committee for IUPAC (1973–present); Associate Member of the Food Contaminants Commission (1973–1978); Titular Member of the Food Chemistry Commission VI.1 (1979–1987); Vice-Chairman of the Food Chemistry Commission VI.1 (1983–1987); Member of the Applied Chemistry Division (1987–1997) and Vice-President (1989–1991); Member of the Bureau (1991–1995); President of the Applied Chemistry Division (1991-1995); Member of the Division Committee of the Division of Chemistry and the Environment (1996-1997); Elected Member of the Bureau and the Executive Committee (1996-1999); Member of the Editorial Advisory Board of Chemistry in the 21st Century (1991 - present); Member of the Committee on Publications and Electronic Printing (1996-1999); Member of the Committee on the Teaching of Chemistry (1996-1999); Member of the International Scientific Advisory Committees for the IUPAC Mycotoxin Symposia held in Paris (1976), Lausanne (1979), Vienna (1982), Pretoria (1985), Tokyo (1988), Mexico City (1992) and Rome (1996); Chairman of scientific sessions at most of the IUPAC Mycotoxin Symposia; Member of the Organizing Committee of the 13th IUPAC Symposium on the Chemistry of Natural Products, Pretoria, August 1982, and Chairman of the Finance Committee; Chairman of the Organizing Committee of the Sixth IUPAC Symposium on Mycotoxins and Phycotoxins, Pretoria, 22–25 July 1985 and Chairman of the Finance Committee; Organizing Chairman of the IUPAC Symposium: A Sustainable Environment—National and International Perspectives, Pretoria, December 1996; Member of the South African Delegation to IUPAC Council Meetings at Münich, Germany (1973); Madrid, Spain (1975); Warsaw, Poland (1977); Davos, Switzerland (1979); Leuven, Belgium (1981); Lyngby, Denmark (1983); Lyon, France (1985); Boston, USA (1987); Lund, Sweden (1989); Hamburg, Germany (1991); Lisbon, Portugal (1993); Guildford, UK (1995) and Geneva, Switzerland (1997).

Awards: Raikes Gold Medal of the South African Chemical Institute (1975), Gold Medal of the South African Chemical Institute (1987), CSIR Merit Prize (1987)—top award of the CSIR, Havenga Gold Medal

Prof. Pieter S. Steyn

for Chemistry (1992) from *Die Suid-Afrikaanse Akademie vir Wetenskap en Kuns*, and Friedrich Schweizer Medal (1993) from the International Association for Cereal Science and Technology, Vienna.

Dr Alan Hayes CBE DL BSc(Gen) BSc (Spec Chem) PhD

Date of birth: 12 June 1930, Manchester, UK

Educated in the public system in Manchester including Technical School. Left school at 15 years of age and joined ICI in the Dyestuffs Division as a 'Lab Boy'.

Through study at evening and part time day classes at the Royal Technical College, Salford (now Salford University) obtained a BSc (Gen) 2nd Class and a BSc (Spec Chem) 1st Class, both London University External.

During this period, he had transferred to the Pharmaceutical Division of ICI and after National Service the company sent him to work in Lord Todd's Laboratory in Cambridge, where he obtained a PhD on the subject of 'Synthetic Approaches to Porphrins and Corrins' after two years.

Dr Hayes returned to work in the Chemistry Research Department of the ICI Pharmaceuticals Division and after four years was appointed Senior Scientist, then transferred to Biochemical Pharmacology, where he became Section Manager and then Biochemistry Research Manager after which Manager of Pharmaceutical Formulation, Analytical Development Quality Assurance and Control.

In 1973 Dr Hayes was appointed to the Board of the Pharmaceutical business and after doing service and marketing jobs he was appointed Deputy Chairman with responsibility for all Research, Technical and Medical matters.

In 1979 Dr Hayes was appointed Chairman of the Plant Protection Division of ICI with responsibility for all aspects of Research, Development, Production, Distribution, Marketing and Sales worldwide. By the time he retired in 1992 this business was achieving sales of $1.8bn and spending over $160m on R&D. Dr Hayes was also instrumental in founding ICI's entry into the Seeds Business and the expansion of its bioscience research. For a spell of two years in the period 1983–85 Dr Hayes served as Chief Planner for ICI in its Head Office organization. During his time in Agrochemicals he served two years as the President of the international trade association GIFAP.

Dr Alan Hayes

Since his retirement Dr Hayes has served as a non-executive Director on several Company Boards and also serves as Chairman of a local independent hospital. In addition, he is a member of the Council of the University of Surrey and of its Finance and Professional Training Committees. He is also Chairman of the Research Park Executive at Surrey University. He is Chairman of the Governing Body of the Chichester Institute of Higher Education.

Activity in scientific societies includes being a Fellow of the Royal Society of Chemistry and membership of the RSC's Science Affairs Board and its Finance Committee as well as being Chairman of Trustees of the Staff Pension Fund. Dr Hayes was President of the Society of Chemical Industry for 1994–96.

With regard to involvement in the affairs of IUPAC, this has largely been with the CHEMRAWN Committee and via that as an ex-officio member of the Bureau; Dr Hayes has also served as a member of the UK delegation to the General Assembly on several occasions.

Dr Hayes' first meeting with the Committee was immediately after CHEMRAWN III in the Hague, the Netherlands. Since then, he says, it has been 'a fascinating but at the same time a frustrating experience'. 'I have enjoyed immensely working with my colleagues on the Committee and I do feel that the whole CHEMRAWN enterprise has been well supported by the members of IUPAC and it has been good for the image of IUPAC. I am sure that in the next phase of its development it can go on to even greater achievements, especially if we can collaborate effectively with the international agencies and other international scientific unions. It has been a great privilege to serve as Deputy Chairman and latterly as Chairman of such a hard working and supportive group of colleagues.'

Past-President

The retiring President, Prof. A.E. Fischli (Switzerland), will remain an Officer (Statute 6.1) and a member of the Bureau for a period of two years (Statute 7.2).

Secretary General—No vacancy

Dr E.D. Becker (USA), the present Secretary General, is elected for the period 1996–1999.

Treasurer—Vacancy

Prof. J.M. Ward (UK), the present Treasurer, completes six years (1992–1997) of service, but he has decided not to stand for a final two years (Statute 6.52).

No nomination for Treasurer had been received as at 20 June 1997.

Bureau—Six vacancies (minimum)

According to Statute 7.2 the Bureau consists of the Officers, the Presidents of the Divisions/Sections, together with not less than ten other members elected by Council, who shall be known as 'Elected Members'. At the conclusion of the 38th Council in Guildford, there were ten Elected Members of the Bureau. At the 39th Council the Bureau will make recommendations to Council as to the number of Elected Members (ten or more), who should be on the Bureau for the succeeding two years.

Elected Members are elected for a period of four years, and they are eligible for election for a second period of four years.

No Adhering Organization shall have more than one Elected Member of the Bureau.

Statute 7.2 also states that 'the principle of fair geographic representation of Members shall be taken into account'.

Nominations for Bureau received (as at 20 June 1997) are: Prof. P. Kratochvil (Czech Republic), Prof. G.J. Leigh (UK), Dr E.P. Przybylowicz (USA), Prof. L.K. Sydnes (Norway)—reappointment, and Prof. C.-H. Zhang (China)—reappointment.

Prof. Pavel Kratochvil (Czech Republic)

Prof. Pavel Kratochvil was born in Prague in 1930. Since 1990 he has been the Director of the Institute of Macromolecular Chemistry of the Academy of Sciences of the Czech Republic, one of the major institutes devoted to basic research in polymer science worldwide. He is also Professor of Macromolecular Chemistry at the Institute of Chemical Technology in Prague.

In 1953, he became a Master of Science in Chemical Engineering at the Institute of Chemical Technology in Prague. Until 1957 he was Lecturer on physico-chemical principles of technological processes at the Institute of Chemical Technology in Pardubice. In 1957, Kratochvil joined the Institute of Macromolecular Chemistry of the then Czechoslovak Academy of Sciences, where he has remained. In 1960, he obtained his PhD and in 1968 a DSc, both from the Academy. His main field of activity is the physical chemistry of polymers, particularly the investigation of solution properties of polymers and copolymers, and light scattering from polymer solutions.

Kratochvil is the author of more than 180 original

Prof. Pavel Kratochvil

communications in international journals, ten reviews, one monograph and five contributions to monographs. He has presented about 240 invited lectures and communications at international scientific meetings and lectures at foreign universities and research institutions.

Kratochvil is a Founding Member of the Learned Society of the Czech Republic, Fellow of the Royal Society of Chemistry, UK, and a member of numerous boards, both national and international, among others the Czech National Committee for UNESCO and editorial boards of international technical journals. He is the holder of the Czechoslovak National Prize for Science in 1970 and of the Prize of the Czechoslovak Academy of Sciences in 1977. He has spent his sabbatical leaves as a visiting scientist or visiting professor in Canada, Germany, India, Mexico, Russia, Sweden and the USA.

Within IUPAC, Kratochvil started his activities as an observer in the Commission on Macromolecular Nomenclature in 1977. He was elected a Titular Member of this Commission in 1979 and served as its Chairman from 1985 to 1991. In the years 1985–1995 he was a Member of the Interdivisional Committee on Nomenclature and Symbols. He became a Member of the Macromolecular Division Committee in 1994. He has been closely involved in various IUPAC-sponsored meetings in Prague, including the International Symposia on Macromolecules in 1965 and 1992, being the Chairman of the latter one, and most of the Prague Meetings on Macromolecules (Microsymposia and Discussion Conferences) over the last 30 years. He has acted as the IUPAC official representative at about ten meetings. Kratochvil serves as the Chairman of the Czech National Committee for Chemistry, the IUPAC National Adhering Organization of the Czech Republic.

Prof. G. Jeffery Leigh (UK)

Prof. Leigh was born on 4 September 1934, and is married with two children.

Education and Career: Studied at University of London, King's College, graduating as top student in 1956,

and taking his PhD in silicon chemistry three years later. Appointed Lecturer in Chemistry in the Faculty of the University of Manchester Institute of Science and Technology (UMIST) in 1959, where he remained for six years, though one was spent on a sabbatical year as a CIBA Fellow with Prof. E.O. Fischer at the University of Munich, Germany.

In 1965, he moved to the University of Sussex, to join the Nitrogen Fixation Unit recently established by Prof. Joseph Chatt. As a coordination chemist, he studied the complex chemistry of dinitrogen as a model for the chemistry of nitrogenases. Under his direct supervision the chemistry group at the Unit became the leading laboratory on dinitrogen chemistry, and Prof. Leigh has now published some 250 scientific papers and supervised about 25 doctoral students. He is probably the world's leading authority on dinitrogen complex chemistry. He left the Nitrogen Fixation Laboratory as Deputy Director in 1994, to become the first Professor of Environmental Science in the University of Sussex. His work has been widely recognized, not least by Her Majesty the Queen by the award of an OBE for services to science. He has lectured in universities and at conferences all over the world, in English or in French, German, or Spanish when appropriate.

Related Professional Activities: Prof. Leigh has been involved in editing and publishing for many years, and has acted as a Deputy Editor of the *Journal of Organometallic Chemistry*, and as Chairman of the Editorial Board of *Dalton Transactions.* He has also served on the Boards of *Inorganic Biochemistry, Inorganica Chimica Acta*, and *Reaction Kinetics and Catalysis Letters*. Within the Royal Society of Chemistry, Prof. Leigh was instrumental in setting up the current system of Editorial Boards, and was founder Chairman of the Inorganic Biochemistry Discussion Group. He has also been Vice-President of the Dalton Division of the Royal Society of Chemistry.

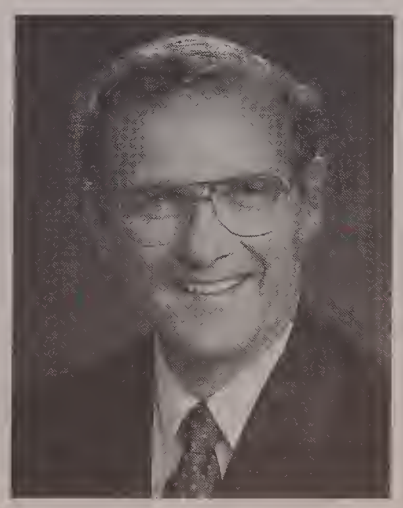
IUPAC Record: Prof. Leigh has been involved in IUPAC activities for about 25 years and has accumulated a wealth of experience at all levels of the organization. He joined the Commission for the Nomenclature of Inorganic Chemistry in the late 1960s, and served as Associated and Titular Member before becoming Secretary for eight years. His major achievement was editing the 1990 version of the Nomenclature of Inorganic Chemistry. Subsequently, he moved to the Inorganic Division Committee, and has been Secretary and Vice-President for four year terms, and is currently finishing a two-year term as President. Not only is he editing an IUPAC book on the Principles of Nomenclature that will be published shortly, but he has also been very active in attempting to resolve the impasse over the names of the transfermium elements.

Dr Edwin (Ed) P. Przybylowicz (USA)

In 1991, after over 35 years with the Eastman Kodak Company, Dr Przybylowicz retired as Senior Vice-President and Director of Research. He joined Kodak as a Research Chemist in the Chemistry Division at the Research Laboratories in September 1956. During his career he had increasing technical and managerial responsibilities in the basic sciences, engineering, product development as well as the Clinical and Copy Products businesses. He became Assistant Director, Kodak Research Laboratories in 1983, was named Director of Research and elected a Senior Vice-President of the company in August 1985.

Dr Przybylowicz has been active in a number of programmes which are focused on the commercialization of technology and in stimulating closer working relationships between industry and academia. He is a Member of the Board of the New York State Science and Technology Foundation, a state foundation which has programmes designed to stimulate the transfer of technology between universities and industry. He is also a Commissioner of the US-Polish Joint Fund for Cooperation in Science and Engineering, a programme which fosters the collaboration of Polish and US scientists. Over the past three years he has co-chaired conferences and workshops on technology transfer in Poland, the Czech Republic and Russia.

Prof. G. Jeffery Leigh



Dr Edwin (Ed) P. Przybylowicz

From April 1994 to March 1996, Dr Przybylowicz was Director of the Chester F. Carlson Center for Imaging Science at the Rochester Institute of Technology. In March 1996 he became Assistant to the Dean, College of Science, Rochester Institute of Technology.

A native of Detroit, Michigan, Dr Przybylowicz received a BS degree in chemistry from the University of Michigan and a PhD degree in analytical chemistry from Massachusetts Institute of Technology. He has published over 20 technical articles and two books in the field of chemistry and photography and holds four patents in related fields.

Dr Przybylowicz was elected a Member of the National Academy of Engineering in 1990 and is active on a number of National Research Council committees. He is an Emeritus Member of the Industrial Research Institute. He also serves on a number of university visiting committees in engineering and the sciences.

Since 1993, Dr Przybylowicz has been a member of the IUPAC Finance Committee where he has helped to strengthen the financial condition of the Union through an improved investment strategy. IUPAC investments are used to keep the Union's operations stable and progressing towards the goals of the Divisions. His active participation in IUPAC affairs is another indicator of his international interests.

He is recipient of a number of awards. The Rochester Engineering Society awarded him the 1992 Leo East Award as 'Engineer of the Year'. In 1993 he was the recipient of the Greater Rochester Chamber of Commerce 'Civic Award in Science and Technology'; the 1994 recipient of the Distinguished Alumni Award from the University of Michigan, Department of Chemistry. In 1995 he was elected Honorary Member of the Society for Imaging Science and Technology for 'his life-long contributions to the advancement of imaging science and engineering, from his technical contributions at Kodak, to his work to enhance industry/university/government cooperation and to expand education in imaging'. In 1996, he was awarded the Malcolm E. Pruitt Award of the Council on Chemical Research for the promotion of university-industry relations.

He is married to the former Roberta Richardson of Owosso, Michigan, and they have eleven children, seven daughters and four sons. Roberta (Bobbi) has a degree in chemistry-biochemistry and was employed by Dow Chemical Company as well as the Arthur D. Little Company. She is currently a volunteer docent at the International Museum of Photography at the George Eastman House and at the Rochester Museum and Science Center in Rochester, NY. Ed and Bobbi's children work in professional fields ranging from healthcare and education to engineering and chemistry.

Prof. Leiv K. Sydnes (Norway)

Date of birth: 9 July 1948. Married, three children born in 1973, 1975 and 1977.

Education: Cand. mag., University of Oslo, December 1971; Cand. real., Organic Chemistry, University of Oslo, October 1974; Dr. philos., Organic Chemistry, University of Oslo, November 1978.

Employment: Research Associate, University of Oslo, 1974-1978; Postdoctoral Fellow, University of Western Ontario, Canada, 1978-1980; Associate Professor, University of Tromsø, 1980–1986; Visiting Professor, Iowa State University, USA, 1985–1986; Professor, University of Tromsø, 1987–1993; Adjunct Professor, University of Tromsø, 1993 to present; Professor, University of Bergen, 1993 to present.

Research and Scientific Publications: The MSc and Dr.philos. degrees were earned under the supervision of Prof. Lars Skattebøl, University of Oslo, on the basis of theses describing research in the field of *gem*-dihalocyclopropanes.

In Canada he worked with organic photochemistry in the research group of Prof. Paul de Mayo, Photochemistry Unit, University of Western Ontario.

The academic year 1985–86 was devoted to organometallic chemistry, which was employed to synthesize prostaglandin derivatives in the group of Prof. Richard Larock, Iowa State University.

The research is mainly concentrated on organic synthesis with emphasis on cyclopropane chemistry and photochemistry. Many of the problems currently investigated are related to the preparation of biologically active molecules. So far the research has resulted in 77 contributions in publications with a referee system. The research has also been presented in numerous lectures/poster presentations in Norway and abroad (more than 80 since 1987).

In his research Prof. Sydnes has so far enjoyed the cooperation of 34 graduate students, 11 PhD students and one postdoctoral student. Currently his research

Prof. Leiv K. Sydnes

group consists of eight graduate students, and five PhD students.

Over the years considerable financial support has been received from Norwegian research agencies and from Norwegian chemical companies (Norsk Hydro, Nycomed, Borregaard).

Non-scientific Publishing: Since 1976 Prof. Sydnes has also been involved in various kinds of non-scientific publishing related to chemistry. He has written more than 50 articles in national periodicals including book reviews of foreign scientific books, papers about chemistry topics for non-specialists, discussion papers about teaching etc. He has written three books covering laboratory work in introductory and intermediate organic chemistry at university level. He has published ten high-school textbooks in chemistry and two chemical textbooks for chemical colleges. He has contributed one or several chapters to 18 technical or more general scientific reports.

Other Professional Activities: In addition to having been and being involved in a large number of committees and boards at the University of Tromsø and now at the University of Bergen Prof. Sydnes has been engaged in professional activities as follows: Chairman, Division of Teaching, Norwegian Chemical Society 1976–78; Chairman, Northern Norway Section, Norwegian Chemical Society 1981–83; Vice-President, Norwegian Chemical Society 1989–92; President, Norwegian Chemical Society 1992–96. Bureau Member, IUPAC 1993 to present; Member, European Communities Chemistry Council (ECCC) 1994 to present; Member, European Communities Registration Board (ECRB) 1996 to present; Member of the COST D2 Management Committee (Selective Synthesis) 1992 to present; Member, INTAS Assessment Panel, Brussels 1994; Member of the Editorial Board, *Acta Chemica Scandinavica* 1989–1994; Member of the Editorial Board, Norwegian Journal of Chemistry (*Kjemi*) 1986 to present; Organizer of The National Organic Chemistry Meeting in 1988, 1992, 1996; Organizer of The Nordic Natural Product Meeting in Tromsø in 1982; Chairman, Organizing Committee, The National Laboratory and Chemical Fair 1992–93, 1994–95, 1996–97; Chairman of the Board, Unilab Analyse AS 1988–92; Member/Vice-Chairman of the Board, Tromsø Research Park AS 1990 to present.

Awards: Kyoto Institute of Technology Lectureship 1990 and The Thaulow Prize 1995.

Prof. C.-H. Zhang (Chinese Chemical Society, Beijing)

Prof. Cunhao Zhang was born in Tianjin, China, on 23 February 1928. He obtained his BSc from Central University, Nanjing in 1947, and MSc from the University of Michigan, USA, in 1950. He returned to China in November 1950 and has been with the Dalian Institute of Chemical Physics, Chinese Academy of Sciences since 1951, where he was an Assistant Professor from 1951–53, Associate Professor from 1953–62 and Professor of Chemistry from 1962. He was Deputy Director of the Institute during 1978–83, and Director from 1986–90. He was elected a Member of the Chinese Academy of Sciences (CAS), a title of the highest academic prestige in China, in 1980, became a Standing Member of the Chemistry Division of CAS by election in 1983, and was elected Chair of the Division in 1994, a position he still holds.

Prof. C.-H. Zhang

He became President of the National Natural Science Foundation of China in 1991. In 1992, he was elected a Fellow of the Third World Academy of Sciences.

Prof. Cunhao Zhang's research activities began in the early 1950s with heterogeneous catalysis. For five years, his group investigated the fluidized bed hydrogenation of carbon monoxide. This resulted in the development of a highly successful nitrided and alkalized fused iron catalyst.

His major research accomplishments have also included valuable contributions to combustion and short wavelength chemical lasers, and to the chemistry of excited molecules, in particular for the development of double resonance multiphoton ionization spectroscopy in probing ultrashort-lived and/or high-lying rovibronic states and in the study of quantum-state specific energy transfer dynamics of excited molecular species.

Prof. Cunhao Zhang has been an invited speaker at various universities and research institutions throughout the world including Germany, Japan, Republic of Korea, the Netherlands and the USA. He has also presented lectures at various international conferences, notably the San Francisco IQEC in 1986 and the 13th ICCE, San Juan, in 1994. He was a CSCPRC Scholar sponsored by US NAS to MIT, UC Berkeley, USC and UCLA in 1985 and a Ho Sin Hang Professor of Chemis-

try at the Chinese University of Hong Kong in 1996.

He holds part-time professorships at universities in several Chinese cities including Beijing, Nanjing and Fudan and is on the Editorial Boards of several journals including *Spectrochimica Acta* and *Chem. Phys. Letters*.

Prof. Cunhao Zhang is an Associate Editor of *Science (China), Chinese J. Chem. Physics* and *J. Molecular Science (China)* and before 1994, a Standing Council Member of the Chinese Chemical Society. He is also a Member of the Optical Society of America and an Associate Member of the IUPAC Commission on Molecular Structure and Spectroscopy. He was elected Vice-President of the China Association for Science and Technology in 1991 and again in 1996.

Report of the International Union of Pure and Applied Chemistry:1996

Mo Williams
Executive Secretary

As a non-General Assembly year, the business of the Union in 1996 was conducted through meetings of the Executive Committee (Oxford, April) and the Bureau (Oxford, September). The membership remained unchanged at 41 NAOs.

Consideration of the future scientific policy of the Union continued through a regional 'brainstorming' session in the USA (Belmont, June). Some 12 academic and industrial chemistry leaders from North America participated in an attempt to develop suitable long-term plans. Follow-up sessions are planned for 1997 in Europe (London, February) and in Asia (Singapore, June). A meeting of the IUPAC Officers with Division Presidents and Vice-Presidents (Frankfurt, March), to consider the recommendations arising from the 'brainstorming' sessions and the 1997 Vice-Presidential Critical Assessment.

Having resolved in 1995 to reconsider its earlier decision, by adopting the 1994 recommendations on names and symbols for the transfermium elements as provisional, the Union duly invited public comment during January–May 1996. The submissions were considered by the Commission on Nomenclature of Inorganic Chemistry (Chestertown/Maryland, August) and revised recommendations for elements 104–109 were referred for comment by the three laboratories concerned in the discovery of TFE. Eventually, the revised recommendations will be presented to the IUPAC Council (Geneva, August 1997) for final approval.

IUPAC considered a number of declarations, particularly the Manila Declaration of 1992 and the Melaka Accord of 1994, on the subject of biodiversity. An IUPAC statement drafted by its Medicinal Chemistry Section, *Preservation and Utilization of Natural Biodiversity in Context of Search for Economically Valuable Medicinal Biota,* was approved by the Bureau and published in the IUPAC journal *Pure and Applied Chemistry (PAC)* (December 1996). Several recommendations were made,

which should be considered by participants when promulgating declarations and enacting legislation on the topic.

Over the past few years, much concern has been expressed about the effect of chlorine and chlorine-containing compounds on the environment. In its capacity as an international non-governmental organization, IUPAC published a *White Book on Chlorine*. The chapters, prepared by 14 experts from throughout the world, critically evaluated various aspects of the subject and are of interest not only to academic institutions, industry, governmental agencies and environmental organizations, but also to the general public. Publication was as an issue of *PAC* (September 1996), and bulk copies were made available to the chemical industry through regional chemical manufacturers associations. The White Book attracted considerable attention, and similar analyses are envisaged of other globally important issues, in which IUPAC can play a role, standing firmly on a scientific foundation independent of governments and industry, by calling on its worldwide network of experts from various fields of chemistry.

CHEMRAWN IX—World Conference on The Role of Advanced Materials in Sustainable Development: Sustainable Production, Use, Disposal and Recycling of Materials—was held in Korea (Seoul, September). It was a follow-up to several earlier CHEMRAWN Conferences on related issues, organized to coincide with the 50th anniversary of the Korean Chemical Society. There were over 360 participants from 17 countries, and the Conference was generally held to have been a success. Important global and multinational problems were identified, such as the role of technology in reducing the ecological load, introduction of renewable energy sources, strategies for selection of and research for ecology-friendly processes, formulation of criteria for estimation of acceptability of current technologies for material production, and effective ways of international cooperation and information exchanges. Two panels on *What New Materials are Needed for Sustainable Development* and *Zero Emissions and Zero Waste Processing for Sustainable Development* focused on problems of primary importance. Proceedings and Perspectives and Recommendations prepared by the Future Actions Committee were published in early 1997.

A reconstituted Committee on Affiliate Membership was assigned the task of considering replacement of the Affiliate Membership Programme as such with elements of priority as identified by the Bureau and Council (Guildford, 1995), including a critical evaluation of the overheads and Secretariat staff costs. It met (Oxford, September) for extensive discussions, with the intention to finalise its recommendations for presentation to the Executive Committee (April 1997). A final proposal will then be submitted to the Council (Geneva, August 1997).

The retirement of the Executive Secretary (March 1997) and other senior staff provided a unique opportunity to move the IUPAC Secretariat elsewhere. After carefully evaluating several possibilities, it was decided to accept an offer to relocate the Secretariat at Research Triangle Park, North Carolina, during 1997 for at least the next ten years, and then to review the location every ten years. A significant financial investment in future information technology equipment and other facilities is required. The opportunity is being taken to update the *History of IUPAC* with a supplement covering 1987–1997 before the Secretariat is relocated.

Meanwhile, an IUPAC Home Page was launched in early 1996 on the Internet (WWW) as a subagent of the UK Royal Society of Chemistry's home page. It provides comprehensive information on the work of the Union, and includes directories of all IUPAC bodies. Chemists will be kept up to date with the Union's meetings and initiatives, training for safety and environmental protection. Also, they can visit chemical industrial WWW sites via hypertext links to the IUPAC Company Associates, and check on publications via the Union's publisher, Blackwell Science. The contents of the home page are being expanded to cover other IUPAC activities, and the possibility of developing IUPAC provisional recommendations via the page is under consideration.

ICSU funding was provided for three IUPAC projects in 1996. A main part of the Education Training project consisted of *The Design and Field Testing of An Environmental Package* by the Committee on Teaching of Chemistry: steady progress has been accomplished, and completion of the work is expected early in 1998.

The Quality Control in Trace and Process Analysis grant was used by the Commission on General Aspects of Analytical Chemistry to organize a meeting (Bologna, August) to discuss the first draft report. A final report is expected in mid-1997. The Water/Aqueous Chemistry grant was used in part to fund a meeting of the Commission on Equilibrium Data (Budapest, July), at which the project on *Complexation Processes in Seawater* was considered. Part I of the report was published (see technical report 5 in Appendix hereto), and a first draft of Part II is expected by mid-1997.

APPENDIX

The following reports on nomenclature, symbols, terminology, and conventions (IUPAC Recommendations 1996) were published during the year:

1 Commission on Chemical Kinetics. A glossary of terms used in chemical kinetics, including reaction dynamics. *Pure Appl. Chem.* 1996, **68**, 149–192.

2 Working Party on Theoretical and Computational Chemistry. Acronyms used in theoretical chemistry. *Pure Appl. Chem.* 1996, **68**, 387–456.

3 Commission on Molecular Structure and Spectroscopy. Symmetry, selection rules and nomenclature in surface spectroscopies. *Pure Appl. Chem.* 1996, **68**, 457–467.

4 Commission on Quantities and Units in Clinical Chemistry and International Federation of Clinical Chemistry. Glossary of terms in quantities and units in clinical chemistry. *Pure Appl. Chem.* 1996, **68**, 957–1000.

5 Commission on Agrochemicals and the Environment. Glossary of terms relating to pesticides. *Pure Appl. Chem.* 1996, **68,** 1167–1193.

6 Commission on Functional Polymers. Terminology for membranes and membrane processes. *Pure Appl. Chem.* 1996, **68,** 1479–1489.

7 Commission on Separation Methods in Analytical Chemistry. Nomenclature for non-linear chromatography. *Pure Appl. Chem.* 1996, **68,** 1591–1595.

8 Joint Commission on Biochemical Nomenclature. Nomenclature of carbohydrates. *Pure Appl. Chem.* 1996, **68,** 1919–2008.

9 Commission on Nomenclature of Organic Chemistry and Commission on Physical Organic Chemistry.

Basic terminology of stereochemistry. *Pure Appl. Chem.* 1996, **68**, 2193–2222.

10 Commission on Photochemistry. Glossary of terms used in photochemistry. *Pure Appl. Chem.* 1996, **68**, 2223–2286.

11 Commission on Macromolecular Nomenclature. Glossary of basic terms in polymer science. *Pure Appl. Chem.* 1996, **68**, 2287–2311.

12 Commission on Macromolecular Nomenclature. Definitions of terms relating to degradation, aging, and related chemical transformations of polymers. *Pure Appl. Chem.* 1996, **68**, 2313–2323.

13 Section on Medicinal Chemistry. Preservation and utilization of natural biodiversity in context of search for economically valuable medicinal biota. *Pure Appl. Chem.* 1996, **68**, 2325–2332.

The following technical reports were published during the year:

1 Commission on Molecular Structure and Spectroscopy. High resolution wavenumber standards for the infrared. *Pure Appl. Chem.* 1996, **68,** 193–208.

2 Commission on Equilibrium Data. Stability constants of metal complexes of amino acids with charged side chains—I: Positively charged side chains. *Pure Appl. Chem.* 1996, **68**, 469–496.

3 Commission on Polymer Characterization and Properties. Critically-evaluated propagation rate coefficients in free radical polymerizations—I. Styrene and methyl methacrylate. *Pure Appl. Chem.* 1996, **68**, 1491–1494.

4 Commission on Microchemical Techniques and Trace Analysis. Analytical methodology for determination of aluminium fractions in natural fresh waters. *Pure Appl. Chem.* 1996, **68**, 1597–1638.

5 Commission on Equilibrium Data. Specific problems in measurement and interpretation of complexation phenomena in seawater. *Pure Appl. Chem.* 1996, **68**, 1639–1656.

6 Commission on High Temperature and Solid State Chemistry. Quantitative analysis of a PbO-SiO_2 glass by electron microprobe. *Pure Appl. Chem.* 1996, **68**, 1657–1663.

7 Commission on Polymer Characterization and Properties. A collaborative study of structure and rheological properties of EVOH/SMA blends produced by reactive extrusion. *Pure Appl. Chem.* 1996, **68**, 1665–1682.

8 Committee on Chemistry and Industry. *IUPAC White Book on Chlorine. Pure Appl. Chem.* 1996, **68**, 1683–1824.

9 Section on Medicinal Chemistry. General features of contracts for natural product collaborations. *Pure Appl. Chem.* 1996, **68**, 2333–2337.

10 Commission on Atomic Weights and Isotopic Abundances. Atomic weights of the elements 1995. *Pure Appl. Chem.* 1996, **68**, 2339–2359.

11 Commission on Thermodynamics. *International Thermodynamic Tables of the Fluid State—Vol. 13: Methane.* Published in book form by Blackwell Science, Oxford, 1996.

12 Commission on Thermodynamics. *Transport Properties of Fluids: Their Correlation, Estimation and Prediction*. Published in book form by Cambridge University Press, 1996.

13 Commission on Thermodynamics. *Heat Capacity of Liquids: A Critical Review and Recommended Values*. Published in book form as Monograph 6 (in 2 volumes) in *J. Phys. Chem. Ref. Data* monograph series by American Chemical Society, Washington, DC, 1996.

14 Commission on Solubility Data. *Solubility Data Series—Vol. 62: Carbon Dioxide in Water and Aqueous Electrolyte Solutions*. Published in book form by Oxford University Press, Oxford, 1996.

15 Commission on Solubility Data. *Solubility Data Series—Vol. 63: Metals in Liquid Alkali Metals—I: Be to Os*. Published in book form by Oxford University Press, Oxford, 1996.

16 Commission on Solubility Data. *Solubility Data Series—Vol. 64: Metals in Liquid Alkali Metals—II: Co to Bi*. Published in book form by Oxford University Press, Oxford, 1996.

17 Commission on Solubility Data. *Solubility Data Series—Vol. 65: Copper (I) Halides* and *Pseudohalides*. Published in book form by Oxford University Press, Oxford, 1996.

18 Committee on Printed and Electronic Publications, *Chemistry for the 21st Century—Reactivity of Solids: Past, Present and Future*. Published in book form by Blackwell Science, Oxford, 1996.

19 Commission on Toxicology and Committee on Teaching of Chemistry, *Fundamental Toxicology for Chemists*. Published in book form by UK Royal Society of Chemistry, 1996.

20 Division on Organic Chemistry, *Highlights in Bioorganic Chemistry: A Symposium in Print, Pure Appl. Chem.* 1996, **68,** 2009–2192.

Thirty-six symposia were sponsored by IUPAC in 1996, namely:

1 26–29 February 1996. 8th International Conference on Phenothiazines and Structurally Related Psychotropic Compounds, Jaipur, India.

2 16–19 April 1996. International Conference on Chemical Physics on the Border of 21st Century, Moscow, Russia. [Proceedings to be published in *Pure Appl. Chem.*, 1997].

3 21–24 May 1996. 2nd International Symposium on Molecular Order and Mobility in Polymer Systems, St. Petersburg, Russia. [Proceedings published as *Macromolecular Symposia* Vol. 113 by Hüthig & Wepf Verlag, Basel, 1997].

4 26–31 May 1996. 2nd International Symposium on Free Radical Polymerization: Kinetics and Mechanisms, Santa Margherita Ligure, Genoa, Italy. [Proceedings published as *Macromolecular Symposia* Vol. 111 by Hüthig & Wepf Verlag, Basel, 1996].

5 27–31 May 1996. 9th International IUPAC Symposium on Mycotoxins and Phycotoxins, Rome, Italy.

6 24–28 June 1996. 11th Bratislava International Conference on Polymers: Thermal and Photo-induced Oxidation of Polymers and Its Inhibition in the Upcoming 21st Century, High Tatras, Slovak Republic. [Proceedings published as *Macromolecular Symposia* Vol. 115 by Hüthig & Wepf Verlag, Basel, 1997].

7 25–29 June 1996. 11th International Conference on Surface Forces, Moscow, Russia.

8 17–20 June 1996. International Symposium on Theoretical and Experimental Aspects of Protein Folding, San Luis, Argentina.

9 30 June–4 July 1996. 11th International Conference on Organic Synthesis, Amsterdam, Netherlands. [*Pure Appl. Chem.* 1997, **69**(3)].

10 30 June–5 July 1996. 11th International Congress on Catalysis, Baltimore, MD, USA. [Proceedings to be published by Elsevier, Amsterdam].

11 7–12 July 1996. 17th International Conference on Organometallic Chemistry, Brisbane, Australia.

12 14–20 July 1996. International Symposium on Sweeteners, Jerusalem, Israel. [Proceedings to be published in *Pure Appl. Chem.* 1997, **69**(4)].

13 14–19 July 1996. 14th International Conference on Chemical Education—Chemistry: Expanding the Boundaries, Brisbane, Australia.

14 15–18 July 1996. 37th Microsymposium on Macromolecules—(Bio)degradable Polymers: Chemical, Biological and Environmental Aspects, Prague, Czech Republic. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1997].

15 22–25 July 1996. 7th International Symposium on Solubility Phenomena, Leoben, Austria. [Proceedings to be published in *Pure Appl. Chem.* 1997, **69**(5)].

16 21–26 July 1996. 18th International Carbohydrate Symposium, Milan, Italy. [Proceedings to be published in *Pure Appl. Chem.* 1997, **69**(7)].

17 21–26 July 1996. 16th IUPAC Symposium on Photochemistry, Helsinki, Finland. [Proceedings to be published in *Pure Appl. Chem.* 1997, **69**(4)].

18 4–9 August 1996. 36th IUPAC Symposium on Macromolecules, Seoul, Korea. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1997].

19 14–17 August 1996. 2nd International Conference on Excitonic Processes in Condensed Matter, Kurort Gohrisch, Germany. [Proceedings to be published in *Pure Appl. Chem.* 1997, **69**(6)].

20 18–23 August 1996. 31st International Conference on Coordination Chemistry, Vancouver, Canada. [Proceedings to be published in *Pure Appl. Chem.* 1997].

21 18–23 August 1996. 11th International Symposium on Carotenoids, Leiden, Netherlands. [Proceedings to be published in *Pure Appl. Chem.* 1997].

22 20–25 August 1996. International Symposium on Macromolecular Condensed State, Beijing, China. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1997].

23 25–29 August 1996. 13th IUPAC Conference on Physical Organic Chemistry, Inchon, Korea. [Proceedings to be published in *Pure Appl. Chem.* 1997].

24 25–30 August 1996. 14th IUPAC International Conference on Chemical Thermodynamics, Osaka, Japan. [Proceedings to be published in *Pure Appl. Chem.* 1997].

25 25–30 August, 1996. 10th International Biotechnology Symposium, Sydney, Australia.

26 1–4 September 1996. International Conference on Environmental Biotechnology, Palmerston North, New Zealand. [Proceedings to be published in *Pure Appl. Chem.* 1997].

27 1–6 September 1996. CHEMRAWN IX: World Conference on Role of Advanced Materials in Sustainable Development, Seoul, Korea. [Proceedings published by Korean Chemical Society, 1997].

28 1–7 September 1996. EUROANALYSIS IX, Bologna, Italy.

29 8–12 September 1996. 14th International Symposium on Medicinal Chemistry, Maastricht, Netherlands.

30 11–13 September 1996. International Symposium on Food Packaging: Ensuring Safety and Quality of Foods, Budapest, Hungary.

31 15–18 September 1996. 4th International Symposium on Characterization of Porous Solids, Bath, UK.

32 15–20 September 1996. 20th IUPAC International Symposium on the Chemistry of Natural Products, Chicago, USA. [Proceedings to be published in *Pure Appl. Chem.* 1997].

33 23–26 September 1996. International Symposium on Polycondensation Related Processes and Materials, Paris, France. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1997].

34 30 September–4 October 1996. 7th International Conference on Multiphoton Processes, Garmisch-Partenkirchen, Germany.

35 13–16 October 1996. International Workshop on Pesticide Use and Environmental Safety in Latin America, Sao Paulo, Brazil.

36 4–8 November 1996. International Symposium on Industrial Applications of Mössbauer Effect, Johannesburg, South Africa. [Proceedings to be published in *Hyperfine Interactions*, 1997].

IUPAC Accounts for 1996

J.M. Ward

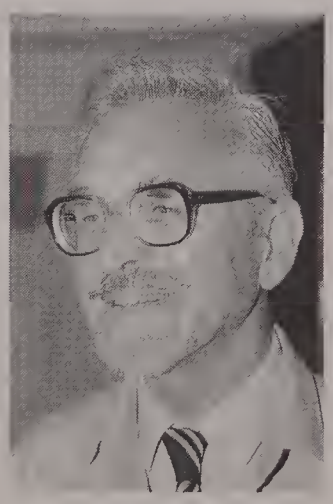
Treasurer's comments

There was an unexpected addition to the Union's funds from Baring Brothers Bank. 'Office Internationale de Chemie', part of the Union when it was created in 1919, had never closed its account with the Bank and so the money plus accrued interest has been paid to us as successors, a sum of USD 343 780. Accountancy rules demand that this sum should go through the Income and Expenses account, so that the accounts show a surplus for 1996 of USD 634 470. But without the 'windfall' the surplus is still USD 290.7k, 129.7k better than budget, a result brought about largely by a Publications surplus of USD 60.8k over budget and an underspend of USD 29.6k on the Affiliate Membership Programme, both results due mainly to a reduction in staff, and so staff costs, during the year. A healthy number of smaller contributions make up the balances.

In 1997 there will be considerable unbudgeted expenses arising from the move of the Secretariat to the Research Triangle Park in North Carolina, as well as recognized additional expenses coming from the extra meetings called to discuss the possible changes to our objectives and methods of working, arising from recent decisions by Council and Bureau. So the 1996 surplus will help to keep what might have been a heavy biennial deficit within reasonable bounds.

Our reserves have increased substantially in value over the year, partly due to the Baring's money and partly due to a good return on our investments. Excluding the Building Fund which now stands at USD 439 605 and the Southern Hemisphere Sinking Fund, the available reserves increased from USD 2451k to USD 3093k during the year. During 1997 another USD 50k will be transferred from the main reserves to the Sinking Fund. The capital needed to equip the Secretariat offices in North Carolina will also be taken from them. Even so, there are still substantial funds available for new initiatives of limited and defined lifetimes, which should arise from the current discussions. We should not be tempted to use the level of reserves as a reason for not keeping our national subscriptions in line with inflation as do all other organizations, companies and retailers.

In conclusion, the 1996 results fully confirm that our finances are now firmly under control and in sound order. We must all determine to keep them so and not slip back to what one might unkindly call the bad old ways.



Prof. J.M. Ward

Auditor's Report

The following is the Report of the Auditors to the IUPAC Executive Committee:

As auditors of the International Union of Pure and Applied Chemistry we have examined the books of account and accounts for the year ended 31 December 1996. Our audit was conducted in accordance with auditing standards promulgated by the profession. We confirm that we meet the legal requirements concerning professional qualification and independence.

Based on our examination, we conclude that the books of account and the accounts are in accordance with Swiss law and the requirements of the statutes.

We recommend that the accounts submitted to you be approved.

NEUTRA TREUHAND AC
Zurich, 19 March 1997

IUPAC Accounts

All amounts expressed in USD

Comparative Balance Sheet[1]

Liabilities	1996	1995
Capital Account	2608 453	2513 028
Accounts Payable[2]	27 811	34 632
Paulo Franzosini Fund	5659	5659
Provisions & Subaccounts[3]	173 155	87 376
Prepaid Subscriptions[4]	36 650	3900
Sundry Creditors	4962	6635
Capital Gains Realized[5]	–3561	–17 919

Unrealized Profit on Securities[8]	272 000	89 381
Excess of Income over Expenses	634 470	113 344
USD	3759 599	2836 036

Assets	1996	1995
Fixed Assets[6]	13 969	22 502
Cash in Banks[7]	261 843	407 228
Marketable Securities[8]	2830 876	2043 746
Building Fund[9]	439 605	302 942
Southern Hemisphere Sinking Fund	50 000	0
Accounts Receivable[10]	15 606	23 368
Subscriptions, etc., Outstanding[11]	147 700	36 250
USD	3759 599	2836 036

Summary of Income and Expenses

	1996	1995
General Expenses net	419 052	–40 849
Publications Income net	200 805	155 732
Affiliate Membership Programme Expenses net	14 613	–1539
To Capital Account USD	634 470	113 344

General Income and Expenses

Income	1996	1995
National Subscriptions[12]	646 010	630 712
Company Associate Service Charges[13]	7010	9000
Observer Country Service Charges[14]	800	1100
Associated Organization Service Charges[15]	1800	1550
Interest & Dividends Earned	115 835	107 854
Other Income	343 780	0
Debit to Capital Account	0	40 849
USD	1115 235	791 065

Expenses	1996	1995
Office Expenses[16]	265 184	290 907
Expenses IUPAC Bodies:		
Standing Committees	68 975	35 384
Divisions[17]	176 222	108 956
General Assembly	8003	329 411
Bad Debts Write Off[18]	0	–44
Bad Debts Provision	11 650	–10 888
Other Expenses[19]	79 896	88 899
Foreign Exchange Differences	–4328	5726
Depreciation	9778	18 786
Provisions: Committed Expenses	80 803	–76 072
Credit to Capital Account	419 052	0
USD	1115 235	791 065

Publications Income and Expenses

Income	1996	1995
Publications: Other Publishers	10 740	13 922
Publications: Blackwell	336 341	331 682
Publications: Secretariat	117	218
BS Support of Publication Activities	20 000	20 000
USD	367 199	365 822

Expenses	1996	1995
IUPAC Secretariat (Pubns.)	144 825	179 965
Chem. Intl. to Symposia	457	351
Miscellaneous Expenses[20]	21 112	29 774
Credit to Capital Account	200 805	155 732
USD	367 199	365 822

Affiliate Membership Programme Income and Expenses

Income	1996	1995
Contributions[21]	82 427	67 544
Royalties Blackwell	2371	3038
Ties & Scarves	58	580
Transfer from General Income & Expenses	0	10 800
Debit to Capital Account	0	1539
USD	84 856	83 501

Expenses	1996	1995
IUPAC Secretariat (AMP)	16 430	28 877
Chem. Intl. & Leaflets	48 935	51 686
Miscellaneous Expenses	4878	2938
Credit to Capital Account	14 613	0
USD	84 856	83 501

Notes to Accounts

1. Accounting Policies

a. Basis of Preparation of Financial Statements

The financial statements are prepared under the historical cost convention.

b. Tangible Fixed Assets and Depreciation

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided on all tangible fixed assets at rates calculated to write off the cost less estimated residual value of each asset on a straight-line basis over its expected useful life as follows:

Fixtures and fittings—over 5 years

Computer hardware—over 5 years

c. Leasing Commitments

Rentals paid under operating leases are charged to the Income and Expenses account on a straight line basis over the period of the lease.

d. Foreign Currencies

Transactions in foreign currencies are recorded at the rate ruling at the date of the transaction. Monetary assets and liabilities are retranslated at the rate of exchange ruling at the balance sheet date. All differences are taken to the income and expenses account, except those incurred in investment transactions, which are taken direct to the balance sheet.

e. Investments

Interest on investment bonds is recognized on a receipts and not an accruals basis.

f. Committed Expenses

The IUPAC Council meets once every two years at the General Assembly to agree budgets for committee operations for the following two years. Starting in 1994, seventy per cent of the budgeted expenses is charged to the income and expenditure account in the first year following the General Assembly and thirty per cent in the General Assembly year.

g. Royalty Income

Royalty income is recognised in the income and expenditure account on a cash received basis.

h. Legal Status

The official headquarters of IUPAC are in Zürich, and the legal domicile of the Union is accepted by the Canton of Zürich as an association under Swiss Law. As such the Union is exempt from any taxation on any net income arising from its activities.

2. Accounts Payable	*1996*	*1995*
List Oxford	23 319	27 462
List New York	4492	7170
	27 811	34 632

3. Provisions and Subaccounts	*1996*	*1995*
Committed Expenses	80 803	0
Bad Debts	20 712	9062
CHEMRAWN Conference Loan Fund	429	7654
Neutra/Audit	9000	9000
Purchases from Blackwells	5832	500
Royal Society Contbn. to Dev. Activs.	9645	11 145
Kratos Grant	136	136
ICSU Grants	33 270	32 408
Lewis Publishers	3613	5004
UNESCO grants	2129	130
Organic Synthesis	1523	1523
Destruction of Chemical Weapons	2621	4621
Oxford University Press—Solubility Data Series	1711	6193
JCAMP-DX Data Standards Project	1731	0
	173 155	87 376

4. Prepaid Subscriptions	*1996*	*1995*
Czech Republic NAO 1997	1300	–
Hungary NAO 1997	3700	–
Netherlands NAO 1997	18 300	–
South Africa NAO 1997	11 500	–
ICC AO 1997	50	–
ISMAR AO 1997	50	–
China CAs 1997	800	–
Hungary CA 1997	450	–
Netherlands CAs 1997	350	–
South Africa CAs 1997	150	–
Croatia NAO 1996	–	1000
Czech Republic NAO 1996	–	1300
Eurachem AO 1996	–	50
ICCC AO 1996	–	50
IZA AO 1996	–	100
Egypt CA 1996	–	450
Hungary CA 1996	–	450
Hungary CA 1997	–	450
Hong Kong OC 1996	–	50
	36 650	3900

5. Capital Gains Realized	*1996*	*1995*
Capital Gains Realized	3383	–32 137
Gain on Building Fund	0	7993
Exchange Differences on Building Fund	–6944	6225
	–3561	–17 919

6. Fixed Assets	*1996*	*1995*
Fixed Assets	96 774	95 529
Depreciation of Assets over 5 Years	–82 805	–73 027
	13 969	22 502

7. Cash in Banks	*1996*	*1995*
USD	–2755	4190
GBP	37 237	15 999
East European Banks	0	17
Money Market Investments	227 361	387 022
	261 843	407 228

8. Marketable Securities

The Marketable Securities are stated at market value in 1995 following a decision by the IUPAC Finance Committee (Minute 4.1(ii)/96, Zürich).

	1996	*1995*
Book Value	3048 481	1954 365
Unrealized Profit	272 000	89 381
Market Value	3320 481	2043 746
comprising Building Fund		
Book Value	396 225	
Unrealized Profit	43 380	
Market Value	439 605	

and General (including Southern Hemisphere Fund of USD 50 000)

Book Value	2652 256
Unrealized Profit	228 620
Market Value	2880 876

9. Building Fund

On the recommendation of the IUPAC Council (Minute 7/91, 36th Meeting - Hamburg), part of the Union's assets have been moved into a building fund, to provide for the eventuality that the need for a permanent Secretariat building becomes pressing.

10. Accounts Receivable	*1996*	*1995*
List Oxford	15 606	13 485
List New York	0	9883
	15 606	23 368

11. Subscriptions, etc., Outstanding

	1996	*1995*
National Organizations	147 050	36 250
Observer Country Service Charges	0	0
Company Associates Service Charges	650	0
Associated Organization Service Charges	0	0
	147 700	36 250
National Organizations (1995)		
Argentina	–	1100
Chile	–	2800
Egypt	5800	5800
Greece	–	3500
Kuwait	–	700
Turkey	–	5650
USA	–	16 700
	5800	36 250
National Organizations (1996)		
Belgium	14 500	–
Brazil	8100	–
Egypt	4900	–
Egypt (CA)	400	–
France	35 100	–
Greece	3800	–
Israel	5000	–
Italy (CA)	400	–
Russia	30 400	–
Slovakia	1000	–
Turkey	3850	–
USA	33 800	–
	141 250	
Service Charges		
Company Associates (1996)		
Egypt	50	–
Italy	50	–
UK	550	–
	650	

12. National Subscriptions	*1996*	*1995*
Received	504 760	594 462
Outstanding	141 250	36 250
	646 010	630 712

13. Company Associate Service Charges

	1996	*1995*
Received	6360	9000
Outstanding	650	0
	7010	9000

14. Observer Country Service Charges

	1996	*1995*
Received	800	1100
Outstanding	0	0
	800	1100

15. Associated Organization Service Charges

	1996	*1995*
Received	1800	1550
Outstanding	0	0
	1800	1550

16. Office Expenses	*1996*	*1995*
IUPAC Officers	2933	9734
IUPAC Secretariat (Non-pubns.)	248 649	269 114
Audit, Bank Fees, Other Charges	13 603	12 059
	265 184	290 907

17. Expenses IUPAC Bodies	*1996*	*1995*
Administration Expenses	19 188	39 642
Meetings other than General Assembly	214 909	104 698
Transfer to CHEMRAWN Account	11 100	0
General Assembly	8003	329 411
	253 200	473 751

18. Bad debts write off	*1996*	*1995*
Bulgaria (AMP)	–	–44

19. Other Expenses	*1996*	*1995*
Contributions to ICSU	20 726	19 785
Representatives Other Organizations	8932	6560
IUPAC Handbook 1994–1995	0	15 654
Chem. Intl. for Members	21 692	21 481
Relocation of Secretariat	1736	0
Appointment of Executive Secretary	15 464	0
Appointment of Information Officer	0	3180
Internet running costs	1303	0
Miscellaneous Expenses	10 043	11 439
Transfer to Affiliates in Developing Countries	0	10 800
	79 896	88 899

20. Miscellaneous Expenses	*1996*	*1995*
BS Travel Grant	20 000	20 000
Other	1112	9774
	21 112	29 774

21. AMP Contributions	*1996*	*1995*
In USD	82 427	66 990
From East Europe	0	554
	82 427	67 544

Subaccounts not Affecting Current Year Income and Expenses

CHEMRAWN	1996	1995
Brought Forward from Balance Sheet	–7654	–15 839
Income from Committee Allocation	–11 100	0
CHEMRAWN IX Contribution	–3000	0
UNESCO Grant Income	0	–1000
Royalties from CHEMRAWN VII Monograph	–1463	–3660
Committee Expenses	22 789	12 844
Net Movement in the Year	7225	8185
Carried Forward to Balance Sheet	–429	–7654

Royal Society Contribution Towards Development Activities	1996	1995
Brought Forward from Balance Sheet	–11 145	–19 922
Income		0
Expenses	1500	8777
Net Movement in the Year	1500	8777
Carried Forward to Balance Sheet	–9645	–11 145

ICSU Grants	1996	1995
Brought Forward from Balance Sheet	–32 408	–35 184
Income	–30 200	–26 200
Expenses	29 338	28 976
Net Movement in the Year	–862	2776
Carried Forward to Balance Sheet	–33 270	–32 408

KRATOS Grant	1996	1995
Brought Forward from Balance Sheet	–136	–136
Income	0	0
Expenses	0	0
Net Movement in the Year	0	0
Carried Forward to Balance Sheet	–136	–136

Lewis Publishers & European Environmental Research Organization (EERO)	1996	1995
Brought Forward from Balance Sheet	–5004	–5004
Income	0	0
Expenses	1391	0
Net Movement in the Year	1391	0
Carried Forward to Balance Sheet	–3613	–5004

UNESCO Grants	1996	1995
Brought Forward from Balance Sheet	–129	0
Income	–2000	–23 000
Expenses	0	22 871
Net Movement in the Year	–2000	–129
Carried Forward to Balance Sheet	–2129	–129

Destruction of Chemical Weapons	1996	1995
Brought Forward from Balance Sheet	–4621	–6434
Income	0	0
Expenses	2000	1813
Net Movement in the Year	2000	1813
Carried Forward to Balance Sheet	–2621	–4621

Organic Synthesis	1996	1995
Brought Forward from Balance Sheet	–1523	–1523
Income	0	0
Expenses	0	0
Net Movement in the Year	0	0
Carried Forward to Balance Sheet	–1523	–1523

Oxford University Press—Solubility Data Series	1996	1995
Brought Forward from Balance Sheet	–6193	–2286
Income	–7719	–6193
Expenses	12 202	2286
Net Movement in the Year	4482	–3907
Carried Forward to Balance Sheet	–1711	–6193
Total from Balance Sheet	–68 814	–86 328
Total Income on Subaccounts	–62 482	–60 053
Total Expenses on Subaccounts	74 489	77 567
Total Net Movements in the Year	12 006	17 514
Total to Balance Sheet	–56 808	–68 814

Movements in Provisions for Year (General Income & Expenses)	1996	1995
Committed Expenses		
Balance Brought Forward	0	–76 072
Net Charge/Credit to Year	–80 803	76 072
Balance Carried Forward	–80 803	0
Bad Debt Write Off		
Balance Brought Forward	–9062	–19 950
Net Charge/Credit to Year	–11 650	10 888
Balance Carried Forward	–20 712	–9062
Neutra/Audit		
Balance Brought Forward	–9000	–8000
Net Charge/Credit to Year	0	–1000
Balance Carried Forward	–9000	–9000
Purchases from Blackwell		
Balance Brought Forward	–500	–564
Net Charge/Credit to Year	–5332	64
Balance Carried Forward	–5832	–500
Total provisions brought forward	–18 562	–104 586
Total provisions carried forward	–116 347	–18 562
Total provisions charges/credits	–97 785	86 024

Securities Account as at 31 December 1996

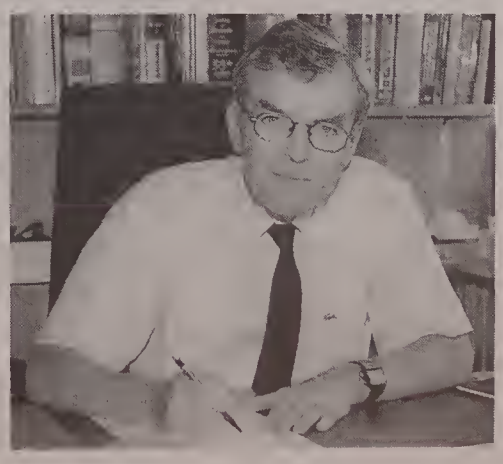
	Currency	Amount	Approx price %	Market value (USD)	Book value at cost	Profit/(loss) since purchase (potential)
Bonds						
6.5% Toyota—4.2.1997	USD	100 000	100.06	100 062.00	97 009.72	3052.28
4.25% General Electric—8.4.1998	USD	150 000	99.56	149 343.00	152 280.56	–2937.56
5.75% Osaka Gas 1993—26.5.1998	USD	100 000	99.69	99 687.00	104 428.40	–4741.40
7% Korea Development Bank—15.7.1999	USD	50 000	101.52	50 758.00	51 162.34	–404.34
7.75% USD Nip. Telegraph—18.11.1999	USD	100 000	104.25	104 250.00	109 652.78	–5402.78
7.25% Salomon Inc Notes—15.1.2000	USD	100 000	101.16	101 155.00	105 108.88	–3953.88
6.125% Southwestern Bell Tel—1.3.2000	USD	100 000	99.36	99 358.00	100 950.39	–1592.39
5 7/8% Euro Ciba–Geigy—23.3.2000	USD	100 000	99.56	99 562.00	100 260.00	–698.00
6.5% USD Abbey Natl Treas—12.5.2003	USD	100 000	100.56	100 562.00	107 913.89	–7351.89
Certificates of Deposit						
CD Bank of America NA Phoenix AZ	USD	90 000	99.87	89 883.00	90 008.98	–125.98
CD World Fin Netwk NB BE Whitehall Ohio	USD	100 000	100.03	100 032.00	100 000.00	32.00
Mutual Funds						
Haussmann Holdings	USD	423	905.04	382 831.00	285 803.81	97 027.19
ML Basic Value	USD	17 148	22.91	392 860.00	285 834.52	107 025.48
ML Euro Equity	USD	15 286	19.40	296 521.98	243 474.53	53 047.46
ML Pacific Equity	USD	25 310	10.37	262 464.00	256 331.96	6132.04
Aetna European Equity	USD	14 777	14.01	207 025.00	183 679.16	23 345.84
Meridian Global Government Fund	USD	9320	10.73	100 003.00	100 365.00	–362.00
Meridian US Emerging	USD	12 235	22.83	279 328.00	270 311.14	9016.86
Permal Asian Holdings	USD	122	1070.84	130 642.00	134 406.95	–3764.95
MLBS USD Fixed Income Portfolio	USD	6230	11.82	73 638.00	69 838.30	3799.70
ML Corporate High Income Portfolio	USD	10 728	9.37	100 516.00	99 659.89	856.11
Grand total securities				3320 480.98	3048 481.20	271 999.78

News

Commission on Biophysical Chemistry: An Introduction

The Commission on Biophysical Chemistry is a recent addition to the Physical Chemistry Division of IUPAC. It came into existence on 1 January 1996. As the chairman of this new Commission I welcome the opportunity to write an introductory note for Chemistry International. By way of introduction it is probably appropriate to give some historical background.

In 1975, IUPAC, IUB and IUPAB decided to create an inter-union Commission on Biothermodynamics. Ingemar Wadsö was chairman and G.T. Armstrong (USA), R.L. Biltonen (USA), J.T. Edsall (USA), H. Gutfreund (UK), W.P. Jencks (USA) and P. Privalov (USSR) were members of this commission. The aim of the commission was to produce guidelines for nomenclature and terminology in the field of biothermodynamics and to organize scientific meetings to this end. In 1985 the Commission on Biothermodynamics was replaced by a 'Working Party on Biophysical Chemistry' which somewhat later was renamed 'Steering Committee on Biophysical Chemistry' (SCBC). This committee was incorporated in the Physical Chemistry Division of IUPAC and given a wider range of responsibilities. It reported to the Physical Chemistry Division Committee, but remained independent in as much as it was not attached to any of the com-



Prof. Helmut Hauser

missions of the Physical Chemistry Division. Ingemar Wadsö, who chaired the former Commission on Biothermodynamics during most of the time of its existence, continued as chairman of the SCBC. Under his guidance a number of biophysically and biochemically oriented projects were initiated and successfully conducted. Working Parties were established to deal with diverse projects such as 'Electrochemical Biosensors' (coordinator: Katsumi Niki), 'Guidelines for Preparation, Characterization and Terminology Concerning Vesicles' (coordinator: Lisbeth Ter-Minassian-Saraga), 'Protein Stability' (coordinator: Brigitte Heinritz), 'Guidelines for Measurements of Redox Potentials of Proteins' (coordinated by Katsumi Niki and carried out as a joint project with the Commission on Electrochemistry), and 'Standardization of Data Bases on Protein Structures Determined by NMR in Solution' (coordinated by Kurt Wüthrich).

When Ingemar Wadsö resigned from the SCBC in 1991, the author was elected chairman of the SCBC. At that time IUPAC's role and service to the chemical society, both industrial and academic, was being questioned, sometimes criticized, and the need for reorientation and restructuring of the Union became clear and was recognized within IUPAC. It was easily foreseeable that the general trend of applying physics and chemistry to problems in biological areas would not only continue but would substantially increase in the future. The working party on 'Hot Spots in Physical Chemistry' created by the Physical Chemistry Division Committee in 1989 delivered two reports in 1991 emphasizing the importance of biophysical chemistry. As a mater of fact, biophysical chemistry was identified as one of the most importanat fields to focus on in the future. All the members of the SCBC were firmly convinced of this fact. We also knew that we were working on timely projects of immediate interest. Most of our members felt that this kind of effort should be stepped up and intensified within IUPAC in the future. The idea of converting the SCBC to an ordinary commission was born. At the General Assembly in Lisbon in 1993, the SCBC submitted a memo to Robert Alberty, then President of the Physical Chemistry Division, urging him to officially propose to the IUPAC Bureau the conversion of our Steering Committee to a regular commission. An official application was filed under Kozo Kuchitsu who succeeded Alberty as President. It took a great deal of effort, intuition, persistency and persuasion as well as the full support of Kozo Kuchitsu, Bob Alberty, Gus Somsen, Mostafa El-Sayed, Ian Mills and other members of the Physical Chemistry Division Committee before our application was approved by the Council at the General Assembly at Guildford in August 1995 and the SCBC was eventually transformed to a regular commission in the beginning of 1996.

The objectives of this new commission, officially now called 'The Commission on Biophysical Chemistry' (Commission 1.7), as laid down in the terms of reference are:

1 To alert the scientific community to the importance of the application of physicochemical methods to biological problems.
2 To highlight areas related to biophysical chemistry where there is confusion regarding definitions, nomenclature, symbols, and related matters and to establish guidelines and recommendations.
3 To establish contacts with other IUPAC bodies with the aim of initiating interdisciplinary joint projects related to biophysical chemistry.
4 To promote communication between the Physical Chemistry Division and other bodies dealing with biology such as IUPAB and IUBMB that deal with biochemistry, biophysics and molecular biology.
5 To contribute to future IUPAC activities in biologically related areas.

These terms of reference were presented and approved of at the IUPAC General Assembly in Guildford in August 1995. The creation of a Commission on Biophysical Chemistry is undoubtedly based on the conviction that the effort within IUPAC on biologically oriented areas will be increasing in the future. Our members also identified the need of alerting other commissions of the Physical Chemistry Division and also other IUPAC Divisions to problems in biology, biochemistry and biophysics. The aim is certainly to help to initiate biological programmes within these commissions and/or as interdisciplinary joint projects between commissions, as proposed in points 3–5 of the terms of reference.

Our commission was created at times of financial constraints which is reflected in the limited number of Titular Members. To start with our commission had three Titular Members: Robert N. Goldberg (USA), who has been vice chairman and secretary, Helmut Hauser (Switzerland), who has been chairman, and Kurt Wüthrich (Switzerland), and six Associate Members: Martin Caffrey (USA), Athel Cornish-Bowden (France), David Eisenberg (USA), Wilfred van Gunsteren (Switzerland), Wolfram Saenger (Germany) and Akiyoshi Wada (Japan). Our proposal to raise the number of Associate Members to nine was granted by the IUPAC Bureau at the end of 1995. Accordingly, Teizo Kitagama (Japan), Terry R. Stouch (USA) and Daniel R. Thevenot (France) joined our commission as Associate Members in the beginning of 1996. Our commission competed successfully for pool Titular Members, and as a result Fred M. Hawkridge, Hans-Jurgen Hinz and Frederick P. Schwarz were assigned to our commission as short-term Titular Members beginning of 1996. Our request for an extension of the terms of these three Titular Members was granted by the IUPAC Bureau in September 1996 so that these three Titular Members will be associ-

ated with our commission until 31 December 1999.

Current activities of the Commission on Biophysical Chemistry are focused on the following IUPAC Programmes:

I 'Electrochemical Biosensors' is coordinated by Daniel Thevenot and a joint project with the Commissions on Electrochemistry and Biotechnology.

II 'Thermodynamics of Enzyme-Catalyzed Reactions' is coordinated by Robert N. Goldberg and Yadu B. Tewari and is a joint project with the Commission on Thermodynamics. The aim of this project was to provide a critical compilation of data on the thermodynamics of enzyme-catalyzed reactions. The data presented were limited to the results of direct equilibrium and calorimetric measurements performed on these reactions under in vitro conditions. This project led to the publication of three major reviews in the Journal of Physical and Chemical Reference Data: 'Thermodynamics of enzyme-catalyzed reactions: Part 3. Hydrolases', *J. Phys. Chem. Ref. Data* 1994, 23, 1035–1103; 'Thermodynamics of enzyme-catalyzed reactions: Part 4. Lyases', *ibid.* 1995, 24, 1669–1698; and 'Thermodynamics of enzyme-catalyzed reactions: Part 5. Isomerases and Ligases', *ibid.* 1995, 24, 1765–1801.

III The project 'Terminology in the Field of Lipid Vesicles (Liposomes): Preparation and Essential Characterization' was initiated and, as mentioned before, originally coordinated by Lisbeth Ter-Minassian-Saraga. After her retirement from the SCBC in 1991 it has been coordinated by Helmut Hauser and run as a joint project with the Commissions on Colloid and Surface Chemistry including Catalists and Biotechnology.

IV 'Standardization of Data Basis on Protein Structures Determined by NMR in Solution' has been coordinated by Kurt Wüthrich. The final document entitled 'Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids' is scheduled to appear in the August issue of *Pure and Applied Chemistry*.

V 'Measurements of Redox Potentials of Proteins' is being carried out in collaboration with the Commissions on Thermodynamics and Electrochemistry. It is coordinated by George S. Wilson and Frederick M. Hawkridge, one of our short-term Titular Members.

VI The project 'A Nomenclature for Lipid Mesophases' was initiated at the General Assembly in Lisbon and is coordinated by Martin Caffrey.

VII 'Recommendations for the Measurement and for the Presentation of Results obtained on Biological Substances with Scanning Calorimetry' was initiated as a joint project with the Commission on Thermodynamics 1994. It is coordinated by Fred P. Schwarz and Hans-Jurgen Hinz who were assigned to this project from the pool of short-term Titular Members.

The first publication submitted recently by our new commission is Kurt Wüthrich's document on the presentation of NMR solution structures. To my mind this project is an example of good and timely service to the chemical community. Solution-state NMR spectroscopy has become an important method of structure determination. Richard Ernst and Kurt Wüthrich of the Swiss Federal Institute of Technology are responsible for the development of the methodology in this field, and needless to say that Kurt Wüthrich is an acknowledged authority in the structure determination by NMR. The method has been used widely in the last decade to determine the structures of peptides, proteins and nucleic acids as well as complexes of peptides and proteins with nucleic acids and other molecules such as, for instance, drugs. A certain consensus has evolved concerning the presentation of NMR solution structures. This has been helped along by issuing guidelines for depositing primary data as well as final structures in protein and nucleic acid data banks and by conventions used by abstracting services. Considering the ever-increasing number of NMR solution structures published in the 1980s, the time appeared to be ripe for the development of generally accepted guidelines for unified nomenclature and reporting standards. With these goals in mind Kurt Wüthrich organized a Working Party (Task Group) as an IUPAC/IUBMB/IUPAB inter-union venture. The project has been supported financially by ICSU and CODATA. The final result of the project is a set of recommendations pertaining to the presentation of NMR data and structures in scientific journals and to the storage of this information in computer-accessible form. This information, in standardized formats, will be freely available to the scientific community. The standardization is important since it is a prerequisite for data exchange. In the course of this project initiated in 1989 the Task Group of eight people has been reviewing previous recommendations of the Nomenclature Committee of IUBMB and IUPAC-IUBMB Joint Commission on Biochemical Nomenclature *(Newsletter* 1992, *Biochem. Int.* 1992, **26**, 567–575) and the Commission on Molecular Structure and Spectroscopy *(Pure Appl. Chem.* 1972, **29**, 627–628, and *Pure Appl. Chem.* 1976, **45**, 219) and has then extended these recommendations in the light of recent developments in the field of biomolecular NMR spectroscopy. This work resulted in several drafts of the recommendations to be issued. These drafts were examined critically by about 50 experts in the field, and were then subjected to two rounds of extensive changes. Modifications and amendments were introduced by the Task Group according to the criticisms and suggestions made by these experts to produce the final document of recommendations.

Regarding the future prospects of our commission we feel that an important assignment given to the members of this commission is to participate in future IUPAC activities in biologically related areas and to contribute to these activities (point 5 of the terms of reference). In this respect our commission may play more than just an ad-

visory role. I believe that the Commission on Biophysical Chemistry is very well equipped for this important task. Our members are chemists who have spent a significant proportion if not a lifetime on research in biological areas. It is this experience that counts and makes all the difference. Future recruitment of members will certainly take care of this point. We need scientists with hand-on experience in research in the life sciences. As the chairman of the Commission on Biophysical Chemistry I would prefer to work on fewer projects in the future than is customary at the moment. I am convinced that what may be called alibi project is not only questionable in terms of usefulness, but is really counterproductive. It is our aim to focus on projects which are very carefully selected and thoroughly screened for what they are worth to the chemical society. To work on fewer projects ensures that our limited resources remain carefully focused. We look forward to close and fruitful contacts and collaborations with other IUPAC bodies. After completing a IUPAC project we regard it as a good sign if the people involved in the work have a convincing and good answer to the final question: Who cares?

IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) and Nomenclature Committee of IUBMB (NC-IUBMB)

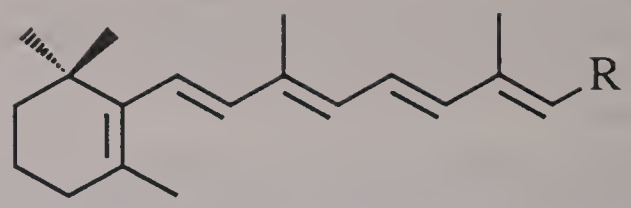
The following are extracts taken from the JCBN and NC-IUBMB joint 1996 newsletter, prepared for publication by Prof. Claude Liébecq, Université de Liège, Belgium.

Vitamin A and retinoids

A document has been prepared by Fritz Weber in consultation with Henry B.F. Dixon and other members of our committees. It has already been published by Fritz Weber (chairman of the former Committee II.1 on Nutritional Terminology of the International Union of Nutritional Sciences) and Athel J. Cornish-Bowden (chairman of our committees) (*Br. J. Nutr.* **74**, 869–870). It is reprinted by permission of the chairman of the Editorial Board of the *British Journal of Nutrition*.

The term 'vitamin A' has been defined as the generic descriptor for all C_{20}-β-ionone derivatives that exhibit qualitatively the biological activity of *all-trans* retinol. The term 'provitamin A' for the carotenoids giving rise to vitamin A is retained.

Chemically, vitamin A belongs to the 'retinoids', defined as a class of compounds consisting of four isoprenoid units joined in a head-to-tail manner. These recommendations also contain the statement: all retinoids may be formally derived from a monocyclic



Formula I: Structure of the parent compound of retinoids

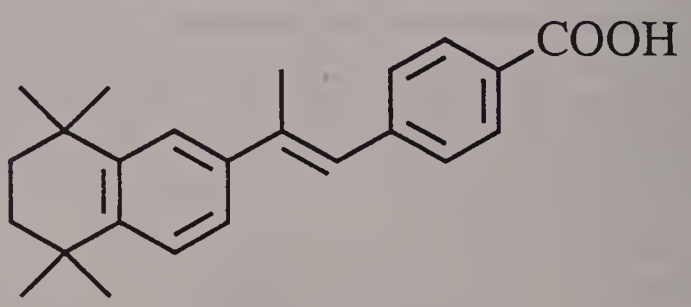
parent compound containing five carbon–carbon double bonds and a functional group at the end of the acyclic portion (Formula I).

The two definitions do not contradict each other. There are, however, certain implications in the words 'vitamin A' and 'retinoids' that should be considered when using the terms.

'Vitamin A' means a group of substances (retinol, retinyl esters, and retinal) with defined biological activities. Further, there are certain metabolites of vitamin A, such as *all-trans* and *cis*-isomeric retinoic acids, that can perform some, but not all, of the biological functions of vitamin A; they are incapable of being metabolically converted into retinol, retinal, etc.

Retinoic acid and some of its isomers and derivatives, together with a number of structurally modified retinoids, have been shown to control cell differentiation in many epithelial tissues and to prevent metaplasia. Some of these substances are used in the treatment of various types of keratinization disorders. Such compounds cannot substitute for vitamin A; indeed some of them even act as vitamin A antagonists.

The term 'retinoids' is widely employed for this class of compounds. This practice arose from an earlier proposal to use the name 'retinoids' collectively for both natural forms and synthetic analogues of vitamin A that are capable of preventing the development of cancer. General usage of this term is, however, misleading for two reasons. Firstly, the customary practice gives the name 'retinoids', which has an agreed definition based on chemical structure, to a class of compounds defined by their biological activity. Secondly, many synthetic members of this class of compounds, the so-called 'arotinoids' or 'retinoidal benzoic acid derivatives' as well as others, are not chemically retinoids. They contain, e.g. aromatic rings replacing either the basic β-ionone type ring structure or unsaturated bonds of the



Formula II: Structure of an 'arctinoid'

tetraene side chain of the retinoid skeleton (Formula II).

We now suggest that the compounds that control epithelial differentiation and prevent metaplasia, without possessing the full range of activities of vitamin A, should be termed 'retinoate analogues'. Although they are usually called 'retinoids', we discourage their designation by a term that has a defined, but different, meaning.

A new term for the group of substances with such antimetaplastic activities may be desirable, especially if it is based on their biological activity. It should not imply a chemical structure because of heterogeneity among the compounds. Proposals for such a term are welcome.

Glycosaminoglycans and proteoglycans

Nomenclature (including abbreviations and acronyms) of glycosaminoglycans (GAG) and proteoglycans (PG) is *ad hoc*.

Older terms such as chondroitin sulfates A, B, or C define major tissue components, but difficulties now occur as hybrid polymers from many tissues do not fit in this system; domain structures present in many tissue GAG are not recognized, and the spectra of modifications due to sulfation and 5-epimerization of D-glucuronic acid (D-GlcA) provide no basis on which to distinguish between, for example, chondroitin and dermatan sulfates (CS and DS). If 10% iduronate (L-IdoA) qualifies chondroitin sulfate to be called dermatan sulfate, are chondroitin sulfate containing 9% iduronate and dermatan sulfate containing 11% iduronate different species?

It is proposed that terminology be based on disaccharide units, which are readily accessible to quantitative analysis, via enzymic digestion. These units are of unambiguous composition and can, for example, be represented by logical abbreviations.

Polymer abbreviations could be two-letter codes, e.g. CS, DS, HS (heparan sulfate) and KS (keratan sulfate). If there is no sulfation, Ch, De, Hp and Ke could be used. They are defined in terms of disaccharide units, thus Ch (chondroitan) is the disaccharide polymer [-4GlcAβ1-3GalNAcβ1-]$_n$, where GlcA is D-glucuronate and GalNAc is *N*-acetyl-D-galactosamine.

DS (currently an abbreviation for dermatan sulfate) consists of not only chondroitin sulfate disaccharides, containing D-glucuronate, but also its 5-epimer, L-iduronate. Probably all 'DS' contains chondroitin sulfate units. In order to avoid confusion about definitions of dermatan sulfate, which imply the complete epimerization of D-GlcA to L-IdoA, the term 'dermochondan sulfate' is proposed, indicating that 'DS' preparations are co-polymeric. The abbreviation 'DS' could be retained for these polymers.

Keratan sulfate consists of repeating -3Galβ1-4GlcNAcβ1- units, sulfated to various extents and in different positions. It belongs to the same polymer group as chondroitin sulfate.

Heparan sulfate is the sulfated polymer of heparan (Hp). Heparan consists of a polymer of the following two disaccharides: -4GlcAβ1-4GlcNAcα1- and -4IdoAα1-4GlcNAcα1-. It is therefore analogous to dermchondan sulfate in containing two uronic acid epimers. There are no names analogous to dermatan or chondroitin in this GAG family.

The abbreviation PG for proteoglycan is in wide use. A rational system should convey information about the protein and the glycan parts. Single names purporting to describe both are certain to confuse, since one part is a gene product and the other is introduced by a post-translational modification. They do not necessarily occur together. It is consistent to use proteochondroitan sulfate (PCS), proteokeratan sulfate (PKS), and now proteodermochondan sulfate (PDS) as abbreviations for proteoglycans with chondroitin sulfate, keratan sulfate or dermatan sulfate chains, respectively. If more than one type of glycosaminoglycan chain is attached to the protein, it is expressed, for example, as P(CS,KS) or P(CS,HS), the dominant GAG being written first. This convention can include quantitative or semi-quantitative information about the GAG, accommodating information on numbers of GAG chains attached to the protein, e.g. P($CS_{70\text{-}100}$, $KS_{10\text{-}20}$, $DS_{7\text{-}10}$).

Protein cores may be viewed as gene products, as amino-acid sequences, as functioning units, or as characteristic shapes (sizes).

Names such as decorin, lumican, aggrecan, syndecan, etc., have been given over the past few years to molecules whose chemistry was known in detail. The names lack chemical information, are inconsistent and should only be used to name the direct gene product.

To emphasize their connection with the gene, rather than with the glycan, the ending 'on' (as in exon, intron, codon) could replace existing 'an', etc. Thus decoron, lumicon, aggrecon, syndecon. A proteoglycan is indicated by adding appropriate GAG abbreviations, e.g. decoron DS, lumicon KS, aggrecon CS,KS.

This complex area of biochemistry would benefit from a structured attempt to rationalize the nomenclature. Comments on the ideas presented here and other suggestions would be welcomed by the nomenclature committees and by John E. Scott of the Department of Chemical Morphology, University of Manchester, Oxford Road, Manchester, M13 9PL, UK (Fax: +44 161 275 4598. E-mail: scott@fs1.ed.man.ac.uk).

The use of 'biochemical equations'

A panel on biochemical thermodynamics, sponsored by JCBN and convened by Robert A. Alberty, has produced a series of recommendations for nomenclature

and tables in biochemical thermodynamics. This report emphasizes the distinction between 'chemical equations', in which the full ionic states of all reacting species should be given in a balanced equation, and 'biochemical equations'. The full charges are often omitted from the equations in routine biochemical presentations. For example, an equation of the form

ATP + acetate = acetyl phosphate + ADP

is commonly used in biochemistry. It makes no attempt to show the full ionization or complexation states or the reactants or to balance charges. It has the advantage that it is written in terms of sums of species and leads directly to the expression for the apparent equilibrium constant K'

$$K' = \frac{[\text{acetyl phosphate}][\text{ADP}]}{[\text{ATP}]\,[\text{acetate}]}$$

which is a function of pH and magnesium ion concentration, as well as T, P and ionic strength. In the above biochemical equation, ATP, ADP and acetyl phosphate are obviously sums of species and, if K' is determined at low pH values, acetate represents the sum of the anion and undissociated acetic acid.

Similarly, it has become common to use NAD^+ and NADH in equations, although both of these are in fact negatively charged at normal physiological pH values, without any attempt to balance charges and hydrogen atoms on other species in the equation. This may make it hard to tell whether a chemical equation or a biochemical equation is intended. In view of such difficulties, the panel has recommended that all indications of charges be removed from biochemical equations and that the full chemical equations, which are written in terms of individual species which may be charged (e.g. H^+, Mg^{2+}, $RCOO^-$, etc.) should be used for those specific cases where thermodynamic behaviour is to be considered.

In writing biochemical equations, it is necessary to use symbols that suggest sums of species and avoid symbols for only one of the species that may be present. Since both chemical equations and biochemical equations are need in biochemistry it is important that the reader should be able to distinguish between these two types of equations at a glance. Failure to make such a clear distinction can lead to hybrid equations that do not have corresponding equilibrium constant expressions and have incorrect stoichiometry. For example, the hydrolysis of 1 mol of ATP to ADP at approximately pH 7 does not produce 1 mol of H^+, as suggested by the equation

$$ATP + H_2O = ADP + \text{phosphate} + H^+$$

but about 0.6 mol. Thus it is recommended that hybrid equations, in which some charges but not others are given, should be avoided as misleading.

The implementation of such recommendations would have substantial implications for the way we have become accustomed to present equations in biochemistry. The views of readers on the desirability of these proposals are being sought.

Development of the enzyme list

Changes in the format: In the future, it is intended that references will be cited at the end of each entry with full title and pagination. In the past, the earliest available reference to a specific enzyme has usually been cited. It is hoped in the future, and starting with new additions to the list, to give more complete and up-to-date references. Good reviews on the properties of any specific enzyme would be particularly valuable citations.

We intend to expand the Comments section for individual enzymes to include information on metabolic significance, relation to other listed enzymes, possible isoenzymes, codification of enzymes of specific interest to clinical chemists, sequence database information, etc. Suggestions for material to include for individual enzymes are always welcome.

Work for the provision of enzyme nomenclature in database format is in progress.

Links with other relevant databases: Several other nomenclature systems and databases are in existence. These include the World Health Organization (WHO) list of International Nonproprietary Names (INNs), the QU number system of the Committee on Nomenclature, Properties and Units (C-NPU) for classifying enzymes of relevance to clinical chemistry, the ReBase of restriction enzymes, etc.

The Enzyme nomenclature database must link to these and the most appropriate ways of doing this are under discussion. Comments and suggestions are welcome.

Deficiencies in the list of enzymes: Advice and suggestions concerning deficiencies or omissions are always welcome. Problems in the classification of monooxygenases, protein kinases/phosphatases, restriction enzymes and other nucleases, are obvious and it would be most helpful if expert groups could be formed to advise on how these might best be classified and unambiguously named.

Submission of new enzymes and corrections to existing enzymes: These can be made on forms available from Keith F. Tipton, Biochemistry Department, Trinity College, Dublin 2, Ireland. Fax: +353 1 677 2400. E-mail: ktipton@mail.tcd.ie

Submissions concerning peptidases should be sent to Alan J. Barrett, Peptidase Laboratory, Department of Immunology, Babraham Institute, Babraham, England

CB2 4AT. Fax: +44 1223 83 7952. E-mail: alan.barrett@bbsrc.ac.uk

Catalytic antibodies: Like enzyme nomenclature, it is proposed that the nomenclature of catalytic antibodies should be based on the reaction catalysed, rather than on structural features. As more than one different 'abzyme' catalysing the same general reaction may be produced, there is clearly a possibility for confusion. However, the catalytic behaviour and specificities may not be identical. Several possibilities are under discussion: they may be included in the Comments section for existing enzymes where they catalyse similar reactions, they might be given EC numbers of they might be given an 'AB' numbering system in a separate list based on the enzyme nomenclature classes. Comments on these possibilities and on the general value of such a listing would be most welcome.

Other catalytic molecules: As in the case of catalytic antibodies the listing of natural and artificial catalytic nucleotides and engineered enzymes with novel specificities could be of use. Advice and comments as to how this could be most helpfully effected are invited.

Other issues covered in the Newsletter include: Naming proteins; Terminology in immunology; Allergen nomenclature; Receptor nomenclature; and Current and future activities.

For further information on the 1996 Newsletter, contact: Prof. Claude Liébecq, Université de Liège, Quai Marcellis 14/011, B-4020 Liège 2, Belgium.

JCBN and NC-IUBMB on the World Wide Web

A Home Page on the World Wide Web has been established for the two committees. This can be found at: http://www.chem.qmw.ac.uk/iupac/jcbn

The Home Page explains the role of the committees and lists its publications, including a WWW full-text version of the recommendations on amino-acid and peptide nomenclature, on steroid nomenclature, on carbohydrate nomenclature and on enzyme nomenclature.

If you have any problems accessing this page, send an E-mail message to: g.p.moss@qmw.ac.uk

Safety Evaluation of Pesticide Residues in Food

The following are three short papers on current issues prepared by the IUPAC Commission on Agrochemicals and the Environment

The aim of the IUPAC Commission on Agrochemicals and the Environment is to critically examine important issues raised by the use of pesticides as related to the health of mankind and the safety of the environment. Topics examined include fundamental aspects of the chemistry of pesticides, their fate in food and the environment; methods of trace analysis; metabolism in animals, plants, water and soil. The Commission works through:

1 Projects which are developed to provide the consensus views of a panel of experts on particular aspects of pesticide chemistry. The reports from these projects are generally published in *Pure and Applied Chemistry*. Large reports are published as monographs. These reports include recommendations for future action either in research fields or in government regulations.
2 Acting as scientific sponsor for the IUPAC Congresses on Pesticide Chemistry which are held every four years.
3 Organizing workshops in developing nations (China, 1988; Thailand, 1992; Brazil, 1996).
4 Liaison with bodies such as WHO, FAO and UNEP to strengthen international collaboration.

The Commission membership comprises up to 18 elected prominent scientific experts. A balance in membership is sought to cover geographical interests, professional affiliations (academic, government research/regulation, commercial R&D) and particular skills in pesticide chemistry. The various nations affiliated to IUPAC can also nominate National Representatives.

The following three short papers summarize current approaches and issues on the safety evaluation of pesticides in relation to their use on human food. The areas of pesticide metabolism and toxicology are subject to stringent government regulation. The testing procedures now followed do give a high degree of assurance that undesirable effects will not occur under worst-case exposure situations. Dietary intake studies are an important means of evaluating the degree to which the population is exposed to pesticides. The more sophisticated current approaches to these studies recommended by IUPAC do provide a high degree of

assurance that the diet is generally very safe with respect to pesticides.

For further information on the Commission and copies of its reports contact: Secretary: Dr Patrick Holland, The Horticulture & Food Research Institute of New Zealand Ltd, Ruakura Research Centre, Private Bag 3213, Hamilton, New Zealand. Tel.: +64 (7) 856 2835; Fax: +64 (7) 838 5085.

I. Metabolism of pesticides in plants and livestock

The use of pesticides to control pests and disease is important for the production of sufficient quantities of safe and affordable food. However, the use of these agents sometimes leaves residues (the pesticide or its degradates) in/on plant parts used as human food or animal feed commodities. These residues may enter the human food chain either directly—through the consumption of treated foods, e.g. grain or fruit, or indirectly—through the transfer of residues to milk, eggs and meat products. To answer the question: 'What is the nature of the chemical residue in/on food or feed items resulting from the use of the pesticide?', plant and animal metabolism studies are carried out. This paper describes the aims and conduct of these studies.

Use of radiolabelled pesticides

The term metabolism generally refers to the chemical transformation of the pesticide which results from natural (metabolic) processes in the biological system under investigation. To measure the total residue, and to provide a means of selectively tracing products derived from the pesticide in the presence of biological material, the studies are carried out using radiolabelled pesticides. The radiolabel, usually carbon-14 or hydrogen-3, is incorporated into a metabolically stable portion of the compound. The use of the radiolabel requires that studies are carried out in controlled areas; for plants this can be either in small field plots or in pots housed in suitable growing environments. This restriction in scale implies that these studies are qualitative and, at best, a semi-quantitative estimate of the fate of pesticides under large scale field conditions.

Plant metabolism

In plant studies, the term 'metabolism' is used in a wider context, to include the formation of all products (degradates) of the pesticide in or on the plant, regardless of whether they result from internal plant metabolic processes, from chemical reactions (hydrolysis and photolysis) or biological processes which occur outside the plant (e.g. microbiological degradation in soil). A plant metabolism study is usually carried out on crops typical of those to which the pesticide will be applied. If the metabolism of the pesticide is the same in plants from three different crop groups, e.g. root, cereal, top fruit, then no further studies are conducted. If different metabolic routes are revealed then studies in a wider range of crops will be initiated. The radiolabelled chemical is formulated and applied to the crop in a similar manner to that used in actual agricultural practice. To define the amount and nature of residues that may be found in rotated crops grown in soil where a previous crop was treated with the pesticide, crop rotation studies are carried out. In these studies, the soil is treated with the radiolabelled pesticide and crops sown 30, 120 and 365 days after treatment. The crops are harvested at maturity and other intervals appropriate to normal agricultural practices, e.g. immature cereals which are fed to livestock as forage or silage.

Livestock metabolism

Studies are carried out in agricultural livestock whenever a pesticide is applied directly to animals or when treated plant commodities are used for animal feed. Typically, the most important species in agriculture are ruminants and poultry, however if the use pattern of the pesticide targets other species then studies would be carried out accordingly. Metabolism studies are carried out in representative species from these groups; usually lactating goats or cows and laying hens are the species of choice. Treatment is carried out to closely approximate expected exposure.

(a) For ingested residues—oral dosing is usually carried out over a period of several days to allow the residues in tissues, milk, and eggs to reach a steady state. The dosing (test) material should reflect the major component of the terminal residue in treated crops. This is frequently the parent compound, however where the parent is not the major component of the residue the test material may consist of a single metabolite, a synthetic mixture of metabolites or plant material resulting from the metabolism studies.
(b) For dermal applications, the radiolabelled chemical is applied, formulated, in a way that reflects the proposed use pattern.

The size of the dose given to the animals is often more than that expected from normal agricultural practice to facilitate the detection, isolation and characterization of metabolites. Samples of milk, eggs and excreta are taken throughout the dosing period. The animals are usually sacrificed within 24 h after the final dose and tissues are taken *post mortem*.

Animal studies must be carried out according to Good Laboratory Practice (GLP) principles (*cf.* the accompanying paper 'The Role of Toxicology in the Evaluation of New Agrochemicals').

Measurement and characterization of the residue

In the case of compounds with a complex structure it may be necessary to conduct two or more metabolism studies with the radiolabel located in different parts of the compound. The use of radiolabelled materials facilitates monitoring of the distribution of the residue throughout the system and provides an estimate of the total residue. By linking radioactive detection with chromatographic separation systems and spectral analysis the individual components of the residue can be isolated, characterized and identified. From this information, the fate of the compound in the test system, i.e. the biotransformation pathway, can be defined.

How the data are used

Once the amount of the total radioactive residues has been determined and the structures of the major metabolites are known, the toxicological significance of the residues can be assessed. If the plant metabolism data indicate that the metabolites formed are both qualitatively and quantitatively similar to those formed in mammals the plant metabolites may be considered to have been tested in animals in the same studies as those performed on the parent compound. If significant qualitative or quantitative differences are found between plant and animal metabolites, additional toxicological data concerning the plant metabolites in animals may be required. The nature and extent of the additional toxicity studies will depend on the nature of the metabolite involved. Using the information from the radiolabelled studies, analytical methods are developed to determine as much of the terminal residue as possible and particularly for those components which are considered of toxicological interest. The development of analytical methods is facilitated using samples from the metabolism studies to optimize the efficiency of the extraction and clean-up procedures.

Conclusions

It is essential that metabolism studies provide an accurate description of the composition of the terminal residues in food and feed items. The nature of the individual components of the terminal residue must be defined before analytical methods, residue levels and toxicity data can be generated. An adequate metabolism study fulfils at least three main purposes;

(i) to identify the composition of the terminal residue in all plant commodities and livestock tissues, milk and eggs.

(ii) to indicate the distribution of the residues, i.e.
(a) in plants, whether the residues are absorbed through roots and foliage or are entirely surface residues and whether the residues are translocated,
(b) in livestock, to indicate the distribution of residues in tissues, eggs and milk and to provide evidence of storage or accumulation in tissues.

(iii) to provide a basis for determining the efficiency of extraction and clean up procedures used in the development of analytical methodologies.

Michael W. Skidmore

Zeneca Agrochemicals, Jealotts Hill, Bracknell, Berkshire, UK. E-mail: mike.m.s.skidmore@gbjha.zeneca.com

Further reading:

Pesticide Metabolism: extrapolation from animals to man. Monograph: Blackwell Scientific Publications, Oxford, 1988 (120 pp).

Use of isolated cells to study the metabolism of agrochemicals in animals. *Pure Appl. Chem.* 1993, **65**, 2299–2312.

Detection and significance of active metabolites of agrochemicals and related xenobiotics in animals. *Pure Appl. Chem.* 1995, **67**, 1487–1532.

II. The role of toxicology in the evaluation of new agrochemicals

The widespread use of agrochemicals as crop protection agents, wood preservatives, vector control agents or industrial/medicinal disinfectants, may result in exposure of man, animals and the environment to these chemicals. Humans may be exposed during production or application and to a lesser extent as consumers of food products which may contain trace levels of residues.

The purpose of this paper is to demonstrate that currently used toxicological test methods and safety assessment procedures safeguard humans against potential adverse effects of agrochemicals. Particular emphasis will be on the assessment of exposure of humans to pesticide residues in foods.

The World Health Organization (WHO) and the Food and Agricultural Organization (FAO) have conducted programmes designed to protect the health of the consumer for more than 35 years. Since 1961 experts from governments and academia have evaluated approximately 230 pesticides (Joint Meetings on Pesticide Residues, JMPR). Monographs are annually issued containing detailed reviews of studies relevant to the establishment of maximum permitted levels of pesticide residues in foods. It should be noted that foods containing residues at the maximum permitted levels are safe for consumption, but the permitted levels are not safety limits.

Strategies of toxicity testing

General principles

All substances exert some degree of toxicity to various forms of life, depending on the exposure level of the

substance. Toxicity studies are focused on the characterization of the precise nature and extent of toxic effects and on the determination of dose levels which do not exert adverse effects (No Observed Adverse Effect Level, NOAEL). Data are generally obtained from experiments with laboratory animals and cultured cells. Occasionally data from occupational or accidental exposure of animals and man to agrochemicals may be used to supplement laboratory animal data. Based on these data and using extrapolation or uncertainty factors, an Acceptable Daily Intake for humans (ADI) may be calculated, i.e. the amount of a substance which may be consumed by humans on a daily basis during the entire life span, without appreciable risk for the occurrence of adverse effects. Comparison of these values with potential exposure of humans to a compound in the environment, including dietary exposure or intake from all foods, will indicate whether the use of an agrochemical may be permitted. Approaches to estimate the dietary intake of pesticide residues in food are described in an accompanying paper 'Dietary Intake of Pesticide Residues'.

Animal studies

The purpose of toxicity studies primarily carried out in laboratory animal species, is to characterize the toxicological profile of a test compound. Choice of the appropriate animal test species is important and ideally species are chosen which respond to a toxic stimulus in a way similar to that expected for humans. Usually rodents (rats, mice, guinea-pigs), dogs and non-human primates are used. The choice of the test animal species depends also on practical considerations such as availability, ease of handling and housing, and availability of background data.

Animal studies must be carried out according to Good Laboratory Practice (GLP) principles. This internationally accepted set of guidelines describes requirements for test facilities, the design of a study protocol and the conditions for performance of experiments, procedures for data recording and reporting, responsibilities for management of a study, and quality assurance procedures. These guidelines are continuously updated according to the latest developments in toxicology and chemistry.

Prior to animal experimentation, test compounds must be characterized with respect to chemical identity, purity and stability. Different types of toxicological studies have been designed in order to characterize a compound:

Pharmacokinetic and metabolism studies—These studies are performed to determine the 'fate' of a compound upon entering the animal body, i.e. absorption, distribution and elimination. In many cases foreign compounds may be converted into substances (metabolites) which are more readily eliminated from the body than the original compound, and therefore information must be obtained concerning the nature of these metabolites. Furthermore, information must be obtained whether a test compound or metabolite accumulates in the body at specific sites and whether the compound interferes with biochemical pathways. Studies of the metabolism of pesticides in plants and livestock are described in the companion paper 'Metabolism of Pesticides in Plants and Livestock'.

(Sub)acute toxicity studies—(Sub)acute studies are performed to screen for potential toxic effects resulting from (unexpectedly) high exposure to a compound. Animals treated with a single or multiple dose of the test compound via the oral, dermal or inhalation route are examined for signs of acute toxicity, skin or eye irritation or sensitization. These studies are of particular relevance for humans involved in the production or application of agrochemicals. These data are used for classification and labeling of compounds.

Long term toxicity studies—These studies are designed to investigate the effects induced by a chemical in animals exposed during a substantial part of their normal life span. Extensive analyses are carried out during and upon termination of the experiment. Blood and urine are analyzed, food and water intake and changes in body and organ weights are recorded, organ functions evaluated, and histopathological analysis of tissues and organs is performed. Insight in the mechanisms of observed toxicity may be obtained from these studies. These studies when properly conducted should provide information on toxic responses caused by increasing dose levels of the test compound and may demonstrate a dose level which does not produce observable adverse effects (NOAEL).

Reproduction studies—Reproduction studies are performed in order to verify that agrochemicals do not affect the reproductive capacity of male and female animals nor affect new borns or young animals. To this end, one or multi-generation studies may be performed with specific attention to potential adverse effects on male and female fertility, incidence of resorptions and abortions, litter size, sex ratio, birth weight and growth of new borns.

Carcinogenicity studies—Of great concern is the potential of certain chemicals to interfere with replication processes of cells, which may lead to the formation of tumours. Specific animal studies are designed to screen for the potency of a test compound to induce tumours. These studies are usually carried out in two rodent spe-

cies orally exposed to various dose levels of the test compound during most of the entire lifespan. Besides evaluation of physiological, clinical and histopathological parameters, tumours are identified on the basis of their histogenic origin. Carcinogenicity studies are performed when:

(i) relevant amounts of residues of a pesticide may be expected in foods,
(ii) structural similarity of the test compound or its metabolites with other known carcinogens has been noted,
(iii) experimental evidence suggests that the test compound may induce early signs of carcinogenicity,
(iv) the test compound has been shown to interact with cellular DNA or chromosomes (mutagenic effects) or
(v) the test compound exhibits new structural characteristics.

Mutagenicity studies—Specific tests have been designed to screen for the genotoxic potency of compounds, i.e. the capacity of a substance to react with the genetic material of living cells (DNA, chromosomes), which may lead to tumour formation or heritable defects. Usually a combination (battery) of different tests is used with bacteria, animals and cells from animal and human origin to detect these types of adverse effects. Results from these studies are used as supplementary information for the establishment of the carcinogenic potential of a compound.

Specialized toxicity studies—Special studies have been designed to assess the potential adverse effects of a chemical on the immune and neural system, and to test for skeletal malformations and other alterations induced by chemicals in foetuses during the period of organogenesis (teratogenic effects). These studies are carried out when the structural properties of a compound or data from toxicity studies indicate potential adverse effects, or in case of compounds with completely new structures.

In-vitro studies—The use of isolated cells, subcellular fractions, or perfused organs and tissues derived from different animal species has become common practice when the toxic properties of agrochemicals are studied. In particular the use of isolated liver epithelial cells (hepatocytes) has been successful in identifying the biotransformation profiles of compounds, and for rapid screening of their toxic potency. Proper use of these systems may complement and reduce whole animal experimentation.

Evaluation of data

The available data provide the basis for the safety assessment of compounds and should include NOAELs for the most sensitive animal species. Knowledge on the comparative metabolism of compounds in animals and man, and on differences in responses to toxic effects of substances, is taken into account when the NOAEL is established. From the NOAEL, normally expressed as mg/kg body weight per day, the Acceptable Daily Intake (ADI) for humans may be calculated, i.e. the amount of a pesticide residue in food and drinking water which can be ingested daily over a lifetime by humans without appreciable health risk:

$$\frac{\text{NOAEL animal studies (mg/kg body weight)}}{\text{SF (safety factor)}} = \text{ADI for humans (mg/kg body weight/day)}$$

In order to extrapolate results from animal studies to humans, safety factors (SF) are applied to allow for potential differences in toxic responses between animal species and man, and to account for possible differences in sensitivity within the human population. Normally a safety factor of 100 is used: 10 (extrapolation between animal species) $\times$ 10 (differences in sensitivity within the human population). However, depending on the available data and their quality, lower or higher factors may be chosen.

The US EPA approach to assess the risks of chemicals is similar to the one described above. Instead of an ADI, a Reference Dose (RfD) is defined derived from the NOAEL by consistent application of uncertainty factors (UF) and of modifying factors (MF). The RfD is a reference point from which potential effects of a chemical at other doses may be estimated. Tenfold UFs are used for extrapolation of experimental results and a MF less than or equal to 10, to reflect scientific uncertainties with respect to completeness of the data base.

Short-term exposure to acutely toxic pesticides such as the organophosphorus or methyl carbamate insecticides, whose toxic action is based on acetylcholinesterase inhibition may not be covered appropriately with the traditional ADI-approach, which assumes a daily exposure to a chemical throughout life. In these cases WHO proposes 'short-term ADIs' or acute Reference Doses (acute RfD), using the same basic principles and methods as for traditional ADIs or RfDs. A NOAEL would be identified on the basis of single or short-term dosing of a chemical.

The ADI concept is not applicable to every type of compound. For instance ADIs cannot be established for those compounds which are slowly eliminated from the body and thus may accumulate. For certain biological effects, such as irreversible bone marrow damage, or genotoxicity a NOAEL may not be identified. In these cases a quantitative risk analysis is made in order to estimate an acceptable risk for the human population.

Since the mechanisms of carcinogenicity are not fully understood, a prudent approach is chosen for the as-

sessment of an ADI. The biological activities of a specific compound are taken into account, and in particular knowledge on the comparative metabolism of the compound in test animal species and humans may facilitate extrapolation of animal carcinogenicity data to humans.

In some cases data on exposure of humans to agrochemicals during production or application or through accidents may be of additional value for the safety evaluation. However in many cases exact exposure levels of chemicals and duration of the exposure are not known.

Conclusions

Principles for the toxicological assessment of pesticide residues in food are based on animal experimentation and other relevant data and are accepted world-wide as the basis for safety evaluation. The ADI concept can be considered as a 'safety-first' approach. Usually large safety factors are applied in establishing the ADI-value, which provides additional assurance that exposure exceeding the ADI-value for short time periods will probably not result in adverse effects. Application of large safety margins is recommended, since humans in practice are exposed to low levels of mixtures of foreign chemicals present in the environment. The experience gained to date indicates that human safety upon exposure to agrochemicals is sufficiently protected. Dietary exposure of humans to residues of pesticides in food resulting from uses according to label instructions is too low to induce adverse health effects in humans. It is important to note that since 1982 established ADIs are being re-evaluated and where necessary revised based on new toxicity data developments in methods of detection, and in improvement of models to evaluate the toxicity of chemicals.

Harry A. Kuiper

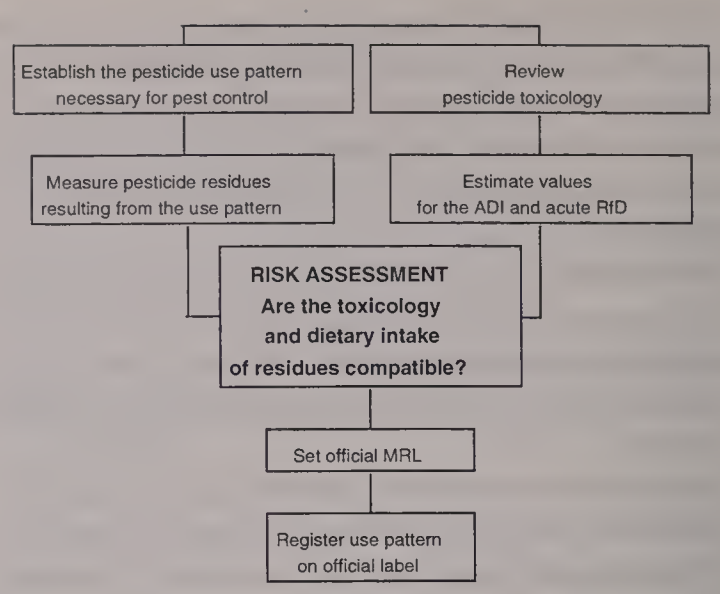
State Institute for Quality Control of Agricultural Products (RIKILT-DLO), PO Box 230 NL-6700 AE Wageningen, the Netherlands. E-mail: h.a.kuiper@rikilt.dlo.nl

Further reading

Principles for the Toxicological Assessment of Pesticide Residues in Food. Environmental Health Criteria 104, WHO-IPCS (1990)

III. Dietary intake of pesticide residues

Decisions on the levels of pesticide residues in foods and the amount of residues likely to be consumed are part of the pesticide evaluation and approval process. The results of two important sets of studies, toxicology studies and studies on likely residues in foods arising from the use of the pesticide, must be reconciled before pesticide uses are approved. Reconciling dietary intakes of residues likely to occur in practice and acceptable intakes derived from toxicology studies is known as the risk assessment process. The place of risk assessment in the pesticide approval process is shown in the simplified diagram (other aspects such as environmental and occupational health aspects are not included here). The conclusions from the toxicological studies and the residue studies must be based on sound science and valid data obtained using convincing experimental methods and should satisfy critical scientific review. An ADI (acceptable daily intake) can be established if the toxicological data are sufficient and valid. The place of toxicology is described in a companion paper 'The Role of Toxicology in the Evaluation of New Agrochemicals'. Estimates of dietary intake of a pesticide residue on a food are obtained by multiplying the level of residue in that food prepared for eating by the weight of that food consumed. The dietary intake of a pesticide residue is then the sum of intakes for those foods where residues of that pesticide occur. Dietary intake assessment of pesticide residues is a difficult task, but is best approached in a scientific manner. We should aim to provide the most realistic estimates possible making the best use of available data. This approach will assist the recognition of genuine problems.


Establish the pesticide use pattern necessary for pest control
Review pesticide toxicology
Measure pesticide residues resulting from the use pattern
Estimate values for the ADI and acute RfD
RISK ASSESSMENT
Are the toxicology and dietary intake of residues compatible?
Set official MRL
Register use pattern on official label

The evaluation process.
***ADI (acceptable daily intake):* estimate of the amount of a pesticide in food and drinking water which can be ingested daily over a lifetime by humans without appreciable health risk.**
***MRL (maximum residue limit):* maximum concentration of a residue that is legally permitted or recognized as acceptable in, or on, a food, agricultural commodity or animal feedstuff as set by Codex or a national regulatory authority.**

Pesticide residues in food

A pesticide residue in food is any substance or mixture of substances in the food resulting from the use of a pesticide, and includes products of biological and chemical breakdown and impurities.

Supervised residue trials are designed to produce reliable data on residues occurring in food and feed commodities under normal commercial practice. The trial conditions are chosen from the efficacy studies, which demonstrate the use pattern (application rate, method, timing, etc) necessary for pest control, but using no more pesticide than necessary.

Because the supervised trials are intended to generate residue data to support the establishment of MRLs (maximum residue limits) we choose the conditions from the efficacy studies which will be the maximum allowable conditions on the registered label. The supervised trials also provide the basic residue data for dietary intake estimation. For dietary intake purposes we are most interested in the residues likely to be present in the edible portion of the food prepared for eating. For enforcement purposes pesticide residue standards (MRLs) are established on the commodity of trade, which may not be the same as the portion which is eaten. A very simple example is fruit with inedible peel such as bananas. The standards of trade are set on the whole fruit, but dietary intake estimates must be made on the residue in the banana pulp. For many pesticides discarding the banana peel also discards most of the residues which might be on the banana. Common household processes such as rinsing and wiping fruit and vegetables remove considerable amounts of surface residues and some pesticides are present mainly as surface residues. However, it is difficult to take this information into account in dietary intake estimations because the degree of cleaning, if any, will be very uneven between households. Vigorous cleaning is often an early step in commercial food processing, e.g. in the milling of wheat and the juicing of apples or tomatoes. If residues are depleted or removed during commercial cleaning or during other parts of the process intake estimations should allow for the reduced residue levels in processed commodities. Some pesticides are destroyed by cooking. Intake estimations make use of this information for commodities such as potatoes, which are always cooked, and for processed food such as canned fruit, vegetables or juices, which are also cooked.

Experience has shown that many pesticide residues concentrate in wheat bran and deplete in flour when wheat is milled. In this example we need to know the consumption of bran and flour (as bread, noodles, etc) separately to make use of such information in the estimation of dietary intake of residues. Metabolism and toxicology studies suggest which of the parent pesticide and its metabolites comprise the residue of concern for dietary intake purposes. This residue is not necessarily identical to the residue used for enforcement purposes on food commodities of trade, but usually the two are identical. The residue for enforcement purposes should be kept as simple as possible because of the difficulties and costs of complex chemical analysis. If the parent pesticide or a metabolite is the main component of the residue it is the best choice for enforcing regulations such as ensuring that a pesticide has been used according to the label. Metabolites of toxicological concern should be included in analyses for total diet studies and for supervised trials being used for intake assessment, even when inclusion is not necessary for enforcement.

Cases occur where cooking produces an undesirable degradation product from the parent pesticide. An example is the production of ethylene thiourea (ETU) from the ethylenebisdithiocarbamate fungicides during heating and boiling phases of food processing. Dietary intake estimations should take into account ETU levels in the processed food even though ETU is not present in the raw commodity. Vigorous washing and cleaning at an early stage of the process substantially reduces the levels of the parent fungicide and the opportunity for ETU production during subsequent cooking.

Chronic and acute intake

Estimates of chronic dietary intake of a pesticide residue on a food are obtained by multiplying the expected or typical level of residue in that food prepared for eating by the average weight of that food consumed daily. The chronic dietary intake of a pesticide residue is then the sum of residue intakes of those foods where residues of that pesticide occur. For chronic intake the long term average or most likely residue in the edible portion is the preferred starting point. In practice the median residue (in the edible portion) from a set of supervised residue trials at the approved use pattern is taken as the starting point estimate of the likely residue for chronic intake. The chronic intake of pesticide residues on minor food commodities is usually insignificant for the reason that, on average, the weight of a minor food consumed is small. It is legitimate to raise the question about large consumption of a food item, particularly a minor food item, on a single occasion, or at least, over a few hours. The question is better answered with the methodology of short term intakes and acute reference doses.

Estimated chronic intake should be compared with the ADI. Estimated short term consumption should be compared with an acute reference dose (acute RfD). The acute RfD should be derived from the toxicology database relating to acute exposure and effects. For acute intake estimates the highest residue in the edible portion from the supervised trials is the best starting point. Residues in individual pieces of fruit or vegetables may need to be considered in some situations because for acute intake the consumer is eating a specific piece, not the average in the consignment.

Chronic intake

= sum of (average consumption of food item x typical residue in food ready to eat)

Compare estimated chronic intake with ADI.

Acute intake

= large portion weight × maximum expected residue in food ready to eat

Compare estimated acute intake with acute RfD

Diets

WHO has information on five cultural diets which may be used in dietary intake estimates at the very broadest level. The five cultural diets are the Middle Eastern, Far Eastern, African, Latin American and European type diets. These cultural diets are based on FAO Food Balance Sheets, which are compiled from a country's food production, imports and exports. Individual countries have much more detailed information derived from specific food consumption surveys on a large number of households or individuals. Food consumption data are then classified according to age, sex, geographic distribution and ethnic background and are available to be used in more accurate dietary intake estimates of pesticide residues for these groups of people.

Individual consumers may eat large portions of specific food items and the food consumption surveys should also capture this information which is needed for the acute or short-term intake estimates.

Total diet studies

The IUPAC Commission on Agrochemicals and the Environment defines a total diet study as pesticide residue monitoring to establish the pattern of residue intake by a person consuming a defined diet. Primary sampling is as for a market basket survey but the samples are further processed as for domestic consumption ie. further trimming and cooking as appropriate to local practice.

Properly conducted total diet studies give the most accurate estimate of pesticide residue intake in the diet. In the total diet study residues in food prepared for eating are measured by chemical analysis. Intakes are calculated from the chemical analysis data and the various relevant diets.

Total diet studies have consistently shown that dietary intakes of residues are well below ADIs. However, total diet studies are limited in their scope because of their cost and complexity. Obviously, they also do not apply to pesticides only recently introduced to the market, or about to be marketed.

Conclusions

The risk assessment of pesticide residue dietary intake is a complex and developing discipline at the centre of the pesticide approval process. It is the link between the toxicology and residue studies. It has become more formalized and has attracted increasing attention in recent years.

Copious quantities of data are available on modern pesticides and we should use the data to make the most realistic estimates for residue dietary intake. We should also recognize that problems as they arise are best solved according to open scientific examination.

Denis Hamilton

Chemical Services, Animal and Plant Health Service, Department of Primary Industries, GPO Box 46, Brisbane QLD 4001, Australia. E-mail: hamiltdj@dpi.qld.gov.au

Further reading

Effects of storage and processing on pesticide residues in plant products. *Pure Appl. Chem.* 1994, **66**, 335–356.

Optimum use of available residue data in the estimation of dietary intake of pesticide residues. *Pure Appl. Chem.* 1997, in press (June issue).

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in The *IUPAC Handbook 1996–1997*. The IUPAC Secretariat has been notified of the following changes:

Prof. Arnošt Kotyk (Chairman, JCBN) Institute of Physiology, Akademie véd Ceske Republiky, Vldenská 1083, CZ-142 20 Prague 4, Czech Republic. Tel.: 42 0 (2) 475 25 56; Fax: 42 0 (2) 471 22 53; E-mail: kotyk@sun1.biomed.cas.cz.

Dr Anders Kallner (President, Clinical Chemistry Section, VII.C), Tel.: +46 (8) 5177 4943; Fax: +46 (8) 5177 28 99; E-mail: Kallner_A/cc@cc.ks.se

Prof. Irina P. Beletskaya (Chairperson, EAB-21st Monograph), E-mail: beletska@elorg1.chem.msu.su

Prof. Rolf D. Schmid (Chairman, COB), Institut für Technische Biochemie, Universität Stuttgart, Allmandring 31, D-70569 Stuttgart, Federal Republic of Germany. Tel.: +49 (711) 685 3193/3192; Fax: +49 (711) 685 3196/4569. E-mail: rolf.d.schmid@rus.uni-stuttgart.de.

Dr Robert D. Vocke (Secretary Commission II.1) A-23 Physics Building, Analytical Chemistry Division, National Institute of Standards and Technology, US Department of Commerce, Gaithersburg, Maryland 20899, USA. Fax: +1 (301) 869 0413; E-mail: vocke@nist.gov.

Dr Margaretha Sluyters-Rehbach (Secretary, Commission I.3), Fax: +31 (30) 253 7483.

Conference Reports

CHEMRAWN IX

World Conference on the Role of Advanced Materials in Sustainable Development, Seoul, Korea, 1–6 September 1996

The UN Conference on Environment and Development held in Rio de Janeiro in 1992 alerted world-wide attention to the effective and wasteless use of materials and energy, zero emission and zero-waste production, and systematic recycling for sustainable development. These strategies are now having a significant impact on the environmental policies of governments and are bringing about change in industrial and economic structure as well as to international trade.

In Korea, the need for reconsideration of mass production at any price and for sustainable development to preserve the environment has been widely felt. CHEMRAWN IX was organized to offer a chance to examine industrial and economic activities of the present day world and to search for effective ways of achieving zero emission and zero waste production.

The CHEMRAWN IX World Conference was held at the Sheraton Walker Hill Hotel, Seoul, Korea, 1–6 September 1996. The Conference consisted of four sessions: Communication, Transportation, Construction and Energy. Academics, scientists and industrialists came to examine and analyze current production technologies and their impacts on the environment. Recycling methods, development of ecologically friendly materials, improving production processes, exchanging information and policy making were all discussed.

Organizing Committee Chairman Dr Min Che Chon gave the opening address, which was followed by congratulatory speeches by Dr A. Hayes, Chairman of the IUPAC CHEMRAWN Committee, and Prof. Saburo Nagakura, President of the Kanagawa Academy of Science & Technology, welcoming remarks by Prof. Sang Chul Shim, President of the Korean Chemical Society, and a Future Actions Committee report by Prof. Young Bok Chae, Chairman of the CHEMRAWN IX Future Actions Committee.

Among the distinguished lecturers were Sir John Meurig Thomas of the Royal Institute of Great Britain and Peterhouse, University of Cambridge, UK, who lectured on 'The Crucial Role of Catalysis in Sustainable Development'; President Jun-ichi Nishizawa of Tohoku University, Japan, who lectured on 'Needs and Seeds for Revolutionary Technology Towards Sustainable Society; the former IUPAC President Prof. C.N.R. Rao of the Advanced Scientific Research & Indian Institute of Science, who lectured on 'The Impact of New Emerging Areas of Solid State Science on the Development of Advanced Materials: Three Case Studies'; and President Charles O. Holliday of DuPont Asia Pacific, who talked about 'Policy and Practical Issues in Sustainable Development: an Industrial Perspective on Opportunities and Responsibilities'.

Among speakers from Korea, President Chung Wook Suh of Korea Mobile Telecommunication talked about 'Wireless Telecommunications in Korea'; Vice-President Sang Bok Hong of Pohang Steel Corporation spoke about 'The Korean Steel Industry and Development'; Dr Han Jung Kim, Director of the Research Institute, Korea Electricity Corporation, talked about 'Issues in Materials Research for Electric Power Generation and Distribution—Perspective of Korea Electric Power Research Institute'; Vice-President Chong Gil Lee of Samsung Electronics talked about 'The Present and Future of the Korean Semiconductor Industry'; and Dr Dae Un Lee, Director of the Research Institute, Hyundai Automobile Corporation, spoke about 'The Automobile Industry of Korea and Sustainable Development'.

Perspectives and Recommendations, a report produced by the Future Actions Committee (FAC) in conjunction with all CHEMRAWN conferences, is distributed to all leaders and policy makers in world politics, economics, science and industry, for their use and reference. The CHEMRAWN IX Perspectives and Recommendations, now available from the IUPAC Secretariat at Oxford, identifies seven key findings and makes six recommendations for future actions, as outlined on page 128.

The CHEMRAWN Committee

Seven key findings

1 There is a need for increased understanding and use of life-cycle assessments in making decisions on materials and technologies supporting the objectives of sustainable development.
2 Ways to recycle complex manufactured goods containing advanced materials need to be developed. Designing such goods for recycling may be a top priority.
3 The importance of conservation of and development of adequate water supplies for agriculture and human consumption cannot be underestimated. Shortages will be the source of major conflicts in the future.
4 There are opportunities in the upgrading of locally available materials with small amounts of other materials or processing technologies from outside the region.
5 The opportunities to improve many traditional materials (steel, cement...) are consistent with the goals of sustainable development.
6 A number of advances in energy production can contribute to sustainable development.
7 Catalysis research offers the potential for routes to sustainable production techniques.

Six key recommendations for future action

The Future Actions Committee (FAC) made the following six key recommendations for future action:

1 We should create a 'materials for sustainable development' research and development agenda to guide national funding agencies.

Action: A team from the FAC will develop a special message and background details from the President of IUPAC to National Adhering Organizations urging that the local organizations approach funding agencies with these priorities. The FAC team will also seek other ways to communicate this message (for example, develop a research agenda to take to a funding agency; develop a research partnership between organizations in developed and developing countries; discuss with the Carter Center, Atlanta, Georgia, UNESCO, UNIDO, UNDP and the International Center for Evaluation of Technology. FAC team 1: C.N.R. Rao, P.M. Norling, J. Nishizawa, S.J. Park, A. Hayes, Y.B. Chae and F. Kuznetsov.

2 The FAC supports the need to contribute to the ready transfer of environmental technologies across industries, across nations and across public/private sectors; to increase the focus from control and remediation technologies to avoidance and resource conservation.

Action: To include urging from the IUPAC President as in Recommendation 1. FAC team 1.

3 We urge the protection of Intellectual Property Rights in a way that acts as an important driver for the introduction of advanced material and process technologies that can further sustainable development rather than as a hindrance to increased collaboration for sustainable development.

Action: FAC Team 1 will include this issue in the letter to be developed under Recommendation 1.

4 We plan to develop a programme of technical education related to sustainable development that can be included in future CHEMRAWN conferences.

Action: Follow up in CHEMRAWN X and propose supporting educational efforts of material societies, UNESCO and UNIDO. FAC team 2: The CHEMRAWN X Organizing Committee and selected members of the CHEMRAWN Committee: R. Pariser, P. Moyna and R. Hamelin.

5 We should urge experts to define (in writing) the needs and opportunities in advanced materials to build a better awareness amongst the public of the contributions of chemistry and advanced materials to our society and to sustainable development.

Action: An FAC team will explore a series of IUPAC monographs 'Chemistry in the 21st Century' using materials from papers presented at CHEMRAWN IX. There is also the possibility of a column or articles in selected magazines or periodicals. FAC team 3: Y.B. Chae, Y.S. Sohn, J.M. Thomas, F.A. Kuznetsov and M.C. Chon.

6 We will urge that where awards are given, special recognition be given to advances in developing materials that contribute to sustainable development.

Action: The FAC will develop a plan to: (i) approach existing award groups and make nominations; (ii) propose that organizations establish such awards; (iii) raise awareness within IUPAC (and other groups) of the existence of such awards. FAC team 4: K. Taylor, J. Economy and A. Tcheknavorian-Asenbauer.

Min Che Chon
Chairman of the Organizing Committee
IUPAC CHEMRAWN IX

Dr Min Che Chon

Copies of the CHEMRAWN IX: Technical Proceedings may be ordered from the Korean Chemical Society, 703 Korea Science & Technology Center, 635-4 Yeogsam-Dong, Kangnam-Gu, Seoul 135-703, Korea.

ACS/IUPAC/CMA/EPA Collaborative Symposium, San Francisco, California, USA

The 213th National Meeting of the American Chemical Society (ACS) held in San Francisco included a collaborative symposium between the ACS, IUPAC, the US Chemical Manufacturers Association (CMA), and the US Environmental Protection Agency. It was held at the San Francisco Hilton and Towers Hotel on 14–15 April 1997 and entitled *Green Chemistry/Environmental Sustainable Manufacture as a Competitive Advantage*.

San Francisco is a fine city on the Western seaboard of the USA. In American standards, it is petite, only 7 miles in length. This city, by the Pacific Ocean Bay, is a town bursting at the seams. Within its watery boundaries lie many neighbourhoods, all with their own charms, peculiarities and even weather conditions.

The Hilton Hotel, the base for this symposium, is at the geographic 'Grand Zero' in the heart of the city's luxury shopping and hotel district.

The symposium was attended by about 150 delegates. It took the form of a number of high-level addresses which were followed by six sessions. These sessions were opened by moderators, and were followed by a panel discussion from three or more internationally respected experts which concluded with an audience, question-and-answer period.

Purpose

The purpose of the symposium was to ensure society of a standard of living acceptable to an increasingly industrial world without danger to the environment or risk to worker health and society. It focused on manufacturing activity and not agricultural activity, except for agriculture as a consumer.

The principal objectives included:

- Encouragement and suggestions for development of environmentally sustainable processes;
- Proposals for competing in the domestic and global market place; and
- Recommendations to government, international and professional agencies, on ensuring safety and environmental protection.

Overview

With the rapid development of new and changing technologies, industrial products and practices inevitably generate materials potentially hazardous to public health and the environment.

Regulation is designed to balance the progress of the chemical and allied industries with the life-sustaining needs of the environment. This concept of sustainable manufacture has become one of the most important challenges for the chemical process industry and has offered the potential for some of the greatest rewards in an increasingly competitive market.

The chemical process industry has often perceived environmental and health regulation as a barrier to productive research and development (R&D). The symposium discussed the relevant issues and recommended methods by which regulations may serve as an aid to competition. Regulation can be viewed as both an incentive and disincentive world-wide.

The symposium was based on six moderated sessions:

- Product development in the chemical industry;
- Risk-based decision-making;
- Business needs in environmentally sustainable manufacture;

San Fransisco hosted the 213th National Meeting of the American Chemical Society

- Human health and environmental health issues;
- Governmental incentives and disincentives; and;
- Implementation in industry.

Keynote lecture

This was delivered by Profs Frank Sherwood Rowland and Mario Molina, 1995 Nobel Prize recipients. They described Atmospheric Chemistry with particular reference to chlorofluorocarbons (CFCs), which were formerly used as a replacement for ammonia and sulfur dioxide in domestic (and other) refrigerators. One part in 10^{12} can cause ozone layer depletion.

The basic chemistry involved is:

$$CCl_3F + UV\ (light) \rightarrow Cl + CCl_2F$$
$$CCl_2F + UV1\ (light) \rightarrow Cl + CClF$$
$$Cl + O_3 \rightarrow ClO + O_2$$
$$ClO + O \rightarrow Cl + O_2$$

Summing $O + O_3 \rightarrow O_2 + O_2$

Ozone deficiency was first observed in the Antarctic in the early 1980s.

In the early 1990s the Montreal Protocol was adapted by a number of Governments but was much too weak and has now been strengthened.

There are considerable problems with developing countries; where the situation has been assisted greatly by the UN Agencies by careful use of multilateral funds. The UN also provides the much needed technical assistance, especially in the least developed countries which have recently introduced domestic refrigerators.

Prof. Molina concluded by saying that unless we make far better use of the limited resources we shall need a planet of three times the size of the Earth.

Prof. Frank Sherwood Rowland gave a very rapid outline of the chemistry involved stressing the importance of the Dobson Spectrometry. He stressed that ozone depletion was first observed in October 1984. The Antarctic vortex has on many occasions now stretched as far as South America, and this is most likely to cause DNA absorption of UVB. This leads to thiamine coding errors due to the formation of cyclobutane pyridine dimers. In countries such as Hawaii, direct sunlight exposure should now only be four minutes instead of the previous twelve minutes.

Prof. Mario Molina

The revised Montreal Protocol is now offering effective solutions but the effects from CFCs will be present until at least the end of the 21st century. This will lead to effects on all biological species.

For the future, Governments and the UN agencies will need to react far more quickly to give higher priority to such early warning of adverse effects having the magnitude of ozone depletion.

Keynote industrial address

The first item of the Industry Forum Breakfast attended by the moderators, panelists and invited guests was the keynote address delivered by Victoria Haynes, Chief Technical Officer of BF Goodrich.

She stressed the need for 20-20 vision and that both sustainability and the need to invest heavily in research and developments were assets for the chemical industry and that these were major corporate matters.

Excellent customer and supplier relations were essential. Sustainability leads to increased productivity and to enhance economic values.

Green Chemistry is a market issue as it leads to, amongst other issues, low waste generation; the chemical industry, including that in the developing countries, cannot be involved in another issue such as Love Canal.

Companies need to comply with the Responsible Care Programmes initiated by the CMA and CEFIC, Montreal Protocols, etc. Developing countries also need to take advantage of the assistance available from the UN Agencies, in particular UNIDO.

Victoria Haynes continued by stressing the importance of the real status of endocrine disrupters and the need for a well balanced report by a well-recognized international body.

There are major technical challenges to be won, including those in chemical science, manufacturing and engineering.

Major products, even in 1997, are manufactured largely by classical methods. There should now be sustainable processes and products using new synthetic procedures, e.g. catalysis, biotechnology, etc. Novel synthesis involving biology and physics were essential.

She highlighted the need for partnerships between academia and industry and to make more with less; and to know more about manufacturing processes and hence to undertake complex syntheses with far fewer synthetic stages.

Allan M. Ford

There was a requirement in processing chemistry to have improvement in engineering and real time control.

The need for recycling and re-use was paramount and the chemical industry needed to seek far more discriminating activities. Such sustainability activities would increase shareholder returns, especially via good and meaningful Intellectual Property Protection and thus achieve competitive advantages.

The opening remarks were given by:

- **Allan M. Ford**, ACS Division of Environmental Chemistry, in formally opening the conference and who thanked both the organizer Mr Scott Stoogenke and the contributors, stressing that it was very much an IUPAC event.
- **Edward Callahan**, representing the Committee on Chemistry and Industry, gave high regards to the current President of IUPAC, Prof. Albert Fischli, and stressed the importance of the conference organized by the American Chemical Society, IUPAC, CMA and the EPA.

This was the third such conference, the first being held in Basle, Switzerland in 1990 [*Chem. Intl.* 1991, **13**(2), 50]. The second in Japan in 1993 [*Chem. Intl.* 1994, **16**(2), 41]; a fourth would be organized in a Pacific Rim country probably in two years time.

Edward Callahan

Mr Callahan stressed growing importance of biochemistry and sustainability. There were many problems in sustainable development with a considerable number of problems to solve, one of which was the chemical description of the oceans in terms of environmental chemistry.

The chemical community needed to be able to tackle environmental chemical problems when they were initially observed and to ensure that potential input would be achieved much sooner than, for example, the influence of CFCs on atmospheric chemistry. This was a challenge for academia, Governments, chemical manufacturers, the UN Agencies, and not least the professional chemical societies and IUPAC.

The IUPAC address was presented by Prof. Albert Fischli, President of IUPAC

Prof. Fischli delivered a masterful and concise account of the history of IUPAC. In the area of environmental chemistry and sustainability he stressed the importance of the recent collaboration between UNESCO and IUPAC. IUPAC was the only International Union with a Committee on Chemistry and Industry, and hence there was a direct route for academia to collaborate with industrial chemists.

He gave due acknowledgment to IUPAC collaboration with various UN Agencies, including UNESCO, International Programme on Chemical Safety (IPCS) and not least the UN Industrial Development Organization (UNIDO). Due emphasis was given to the sterling work being undertaken by Division VI—Chemistry and the Environment Division.

There was a growing requirement for globalization for a greater activity in industrial rather than pure chemistry within IUPAC. This was achievable with collaboration with UNIDO.

Great emphasis was given to the overwhelming response that had been received from the 'White Book on Chlorine' [*Pure Appl. Chem.* 1996, **68**(9), 1683–1824]. As a future topic of growing public concern, Prof. Fischli indicated that endocrine disrupters would be the subject of a forthcoming 'white book'.

Within developing/industrializing countries, there was an immediate need for training and this should be achievable by IUPAC's ongoing collaboration with UNESCO and UNIDO.

Session A—Product development in the chemical industry

Moderator: Joseph Coates (Coates and Jarratt Inc.).
This symposium explored the broad trends influencing the future of chemistry as a science and its reduction to practical applications. Speakers dealt with individual aspects of the future of the chemical industry in terms of sectorial developments, industrial developments and

some product developments as well as market changes over the next decades. Special attention was given to the very important role of environmental considerations in shaping the future of the industry.

The moderator and three panelists, in developing these topics, stressed the need for the merging of chemical disciplines, e.g. inorganic with organic chemistry and with other natural sciences, in particular biology and physics.

In the future they foresaw major developments being gained from genetics, computer imaging, catalysis, especially the use of enzymes developed from extremeophiles, gas hydrates and hydrogen, as a prime power source, intelligent materials, especially in composites, lubricants and polymers, new fertilizers with micro delivery systems, and the use of nanotechnology.

In outlining Project 2025 they considered that information technology, material technology, genetics, energy technology and environmentalism to be areas for development. There had to be a drive by science and technology to decrease the usage of toxic chemicals.

A competitive advantage was achievable by the use of ISO 14000. There was an increasing public demand in the environment and the non-specialist should be able to gain information via information technology, e.g. the Internet.

The public has a right-to-know in material accounting and its effect on air and water and this was achievable through the chemical industry with IUPAC assistance via libraries and schools.

In this way, increasing accountability in sustainable development was achievable to give competitive advantages.

Session B—Risk-based decision making (co-sponsored by CMA)

Moderator: David Sigman (Exxon Chemical)
This covered:

1 Need for risk and benefit-cost legislation
2 Wise application of judicial review of regulation
3 Improving risk-based data bases
4 Enhancing federal risk guidance
5 Development of comparative risk methodology
6 Development of risk principles
7 Interpretation and application of the precautionary principle

The points stressed by the moderator and three panelists included the priority being given by the CMA in law and policy and the importance of risk assessment and risk management. In view of the growing number of chemicals being synthesized, greater use had to be given to priority setting.

In risk management greater input was required from the informed public. This in turn required improvements in risk communications.

There was a need for basic research, especially the mechanisms by which chemicals react with the environment and interaction with human health.

One of the topics of current concern was endocrine disrupters and the CMA was funding research over the next two years. During the discussion period, the concern for these was highlighted, especially that the chemicals elicited to exhibit endocrine disrupters should be considered very carefully and their criteria specified. There was a very urgent need for the development of a reliable chemical or biochemical test procedure.

The panelists stressed the need for ecological assessment research, especially to support the risk reduction strategies identified within Chapter 19 of Agenda 21.

Session C—Business needs in environmentally sustainable manufacture

Moderators: Balasubramanyan Sugavanam and Ralph (Skip) Luken (UNIDO)
This covered:

1 Definition of Environmentally Sustainable Manufacture
2 Importance of chemicals vs. impact on environment
3 Source reduction vs. end of pipe treatment (Cleaner production)
4 Self regulation vs. enforcement
5 Environmental justice and its relevance
6 Tools used for environmentally sustainable manufacture:
   (a) Responsible care
   (b) Control of substances hazardous to health and environment (COSHHE)
   (c) Life cycle analysis
7 Monitoring:
   (a) Eco-labeling
   (b) Ecotoxicity
   (c) ISO 14000

Balasubramanyan Sugavanam

8 Accountability:
(a) Corporate responsibility
(b) Government responsibility
(c) Responsibility of international organizations
(d) Responsibility of non-governmental organizations
(e) Public role
9 Recommendations

The points stressed by the moderators and three panelists included environmental sustainability, its management and difficulties, especially in the least developed countries. Greater emphasis was needed in upstream environmental sustainable manufacture. Regrettably the concern for the environment, particularly in a number of developing countries, had progressed from bad to worse.

A video demonstrated very clearly the considerable successes that UNIDO had achieved in sustainability in a number of developing countries, emphasizing the achievements in economy, environment and employment.

Major equity concerns need to be addressed, especially as poverty induced poor environmental conditions. With the support of experts having wide international experience, UNIDO was working actively and with an excellent success rate in environmental impact assessment, the use of new technologies and techniques, leading to successful environmental and integrated management procedures.

This was being achieved through life cycle studies, vision, action and eco-efficiency, in turn resulting in an impressive reduction in illness rates and increases in process and product safety.

Session D—Human health and environmental health issues

Moderator: Fred Hoerger (formerly Dow Chemical)
This covered:

1 New Priorities:
(A) Global
(i) Climate change
(ii) Restoration of fisheries
(iii) Biodiversity
(a) Loss of rain forests
(b) Loss of habitat
(B) National
(i) All inclusive health and environmental benefits
(ii) Equitable opportunity for achieving economic environmental, and social well being
(iii) Use, conserve, protect, and restore natural resources
(C) Local (regional, community)
(i) Stop the loss of prime farmland
(ii) Redevelop 'brown' urban areas
(iii) Protect, enhance habitats and biodiversity
(D) Conflicts
(i) Agreement on priorities and allocation of resources between sectors and within sectors
(ii) Reliance on trade-offs and comparative risks and benefits instead of absolute risk and benefit in decision making

2 New Framework for Action:
(A) Research
(i) New priorities and international agenda setting
(a) Long-term approaches
(b) Emerging global problems
(c) Relation between human and natural systems
(d) R&D to improve risk assessment and cost-benefit analysis
(ii) Trends and status of the environment
(iii) Interdisciplinary, international collaboration
(B) Regulatory
(i) Performance-based standards
(ii) Stewardship
(iii) Market-based incentives
(iv) Enhanced product responsibility programmes
(C) Education
(i) Health, environmental content of curriculum
(ii) Accessibility of information
(iii) Lifelong learning
(D) Cooperative, open planning and action at the community level
(E) Information collection, management, distribution
(i) What is needed?
(ii) What is the nature of the system?
(iii) Who funds and manages the system?

3 There is Momentum to Solve the Issues

4 Issues Related to Implementation:
(A) What type of information is needed about important air contaminants?
(B) How do we establish what are the important contaminants in drinking water and ground water and their sources?
(C) Within the framework of NAFTA, what are the important trans-boundary human health problems that need to be addressed?
(D) On a societal basis, how does one balance the priorities for clean air and clean water with the priorities which relate more to ecosystem health (e.g. comparing the priority for decreasing ambient air contaminants to preserving wildlife habitat)?
(E) Can comparative risk studies provide insight for the regulatory/legislative arena, or is the trade-off strictly political?
(F) How can health related agencies and professionals interact with and coordinate their efforts with ecologically oriented agencies and professionals?

The moderators and five panelists reviewed a number of topics of current concern including test methodologies for estrogen mimics, risk assessment methodology and needs for benefit–risk appraisals.

One conclusion was that we were slowly evolving towards a new environmental paradigm—but an evolution which is hampered by existing institutions and counter political and social priorities. Current activities are still hampered by the laws, regulations and mentality of the past two decades and only a small overlap with the vision of sustainable development. The current focus needs included protecting humans from the environment and equally the environment and the ecosystems from humans. There was a need to gain expertise in how to ask the right questions to provide meaningful answers. Increased attention was needed in pragmatic and attainable environmental legislation with an input from the public. This was now achievable through the activities of the International Forum on Chemical Safety (IFCS), the current presidency being held by Canada.

There was a need to achieve sustainability by interaction between environment and societal activities.

One of the panelists reported on a serious area of lack of sustainability, namely warfare in the environment. Whilst the media accentuated human suffering, the dramatic and often irreversible effects to the environment were neglected by the media, mediators and politicians. UNIDO had been active and successful in assisting Croatia by sending an international expert during the conflict to observe, report and recommend remedial action.

Considerable discussion was held on the need for meaningful environmental monitoring, especially in the least developed countries or in areas depredated by warfare. It was recognized that generic testing, such as the use of *Vibrio fisheri* (the Microtox test) had much to offer. Of greater importance was the need for developing/industrializing countries and in particular countries in transition to ensure that their environmental legislation was pragmatic in such a manner as to ensure it was geared to both the country's capabilities in environmental monitoring (and hence the use of generic techniques) and the capability and training of scientists to be able to undertake risk assessments, risk management, leading to risk reduction, and hence chemical safety.

UNIDO had been very active and successful in such areas. One notable example being the establishment of a regional ecotoxicology laboratory in Islamabad, Pakistan, serving the requirements for South-East Asia.

UNIDO also had the foresight to engage the services of a high-level scientist in 1995 to travel to a number of Central and Eastern European countries and selected Arab Stages to report and provide recommendations on Environmental Monitoring of Industrial and Domestic Pollutants and Chemical Safety.

This major assignment led to the implementation of a number of projects on sustainable manufacture with competitive advantages. Funding of these projects was of concern and the meeting was asked to invite tax payers in every country to assist the UN Agencies and, in particular UNIDO, to build on these firm foundations to persuade their Governments to support the sterling work of these Agencies, which over 150 Governments ratified at the Rio Summit (UNCED) in June 1992. This commitment has to be supported to the fullest.

With such provision, real strides forward can be taken to the maximization of risk reduction procedures and sustainability as we enter the 21st century.

Session E—Governmental incentives and disincentives

Moderator: Jean-Jacques Salzmann (Novartis)

This covered:

1 Introduction:

(A) Goal of business and government is a sustainable economy

(i) Balance between growth, competitiveness, employment, and the limited carrying capacity of the environment

(ii) Balance requires shared responsibility between producer, consumer, and legislator

(B) Questions

(i) Is industry willing to improve its environmental performance in the direction of sustainable development?

(ii) Are the financial markers, which press business to maximize shareholder value, open to consider sustainable criteria?

(iii) Are the legislators capable of introducing rules and incentives adapted to the purpose of sustainability?

(iv) Are the consumers willing to change their attitude and behaviour to the needed level of environmental responsibility?

2 Thesis 1:

(A) As long as the environment is still considered as a free and common good, legislation will be necessary.

(B) As long as industry is striving for 'compliance only', new incentives to go beyond and towards sustainability are necessary.

(C) Recommendations

(i) Industry and legislators should enter into a pro-active dialogue.

(ii) They should become partners for solutions towards sustainable regulations and incentives.

(iii) Industry should break down and allocate the environmental costs to their products (Cost-allocation would lead to an internal regulatory instrument).

(iv) Environmental regulations should always be based on a scientific risk assessment and the cost-benefit relation should be demonstrated beforehand.

(v) The 'precautionary principle' should not be misused to prescribe techniques or to ban/phase out products.

3 Thesis 2:

(A) There is a strong discrepancy between the global environmental problems and the political decisions on the local level.

(B) Local environmental protection decisions too often ask for large investments for business with a marginal effect on improving the quality of the environment.

(C) Recommendations

(i) Environmental regulations should be harmonized on an international or at least on a regional level.

(ii) 'Joint implementation' procedures should be enhanced, whereas efforts and investments should be made in these (geographical) areas, where the environmental yield per dollar can be maximized.

4 Thesis 3:

(A) Command and control legislations have only limited effectiveness.

(B) In setting not only the environmental objectives, but also in prescribing the means to reach the objectives, these legislations are hindering innovations and are often unsustainable.

(C) Innovation is for business the main driving force to improve its environmental performance.

(D) Recommendations

(i) The use of a 'policy mix' should be advocated.

(ii) Besides command and control regulations, market oriented instruments and enforceable (negotiated) agreements, which allow a sustainable use of scarce resources and production factors should be used.

(iii) Environmental quality objectives should be set.

(iv) The corresponding regulatory instruments should not only be focused on specific industrial sectors but they should encompass all potential pollution sources.

The moderator and three panelists referred to whether regulations were of assistance or hindrance to the manufacturing industry. It was vital to receive cooperation and not enter into confrontation.

Eco-efficiency was now an achievable goal through training on emissions or discerning use of taxation.

The achievement of wealth and value creation through environmental sustainability was stressed, but it was pointed out that the financial market works against environmental sustainability and investors on the whole do not appreciate environmental issues. Hence, there was a need to convince accountants of the importance and monetary benefits to be attained from environmental sustainable development.

There were requirements for joint projects.

Governments must think globally, especially when dealing with environmental issues, as pollutants do not recognize national boundaries.

There was a need to have far less command and control from government. There was a considerable opportunity for cooperation between industry and regulators with major inputs from bodies such as the CMA, IUPAC and the UN Agencies, leading to trust and cooperation through negotiated agreements, products at the right price, exhibiting eco-efficiency, thus providing shareholders with demonstrable value.

Session F—Implementation in industry

Moderator: Earl Beaver (Monsanto)

The moderator and four panelists reviewed many of the key points from the previous five sessions.

There were needs to be imposed upon the chemical industry from an historic viewpoint; the vision 2020 projects and industrial needs, leading to an objective path forward.

Cost and product quality were key factors for the 21st century.

Competition was of increasing importance, but at the same time, much greater attention had to be given to processes involving toxic and hazardous substances.

Many chemical companies had been very successful in achieving considerable reduction in waste and this was likely to continue in the future.

By 2020 the chemical industry would be a world leader.

Particular aspects of success could be in the enhancement of health, safety and the environment and modeling, especially eco-efficiency models, product development cycles, leading to greater value added products and integration of data bases which was currently not feasible.

Much greater emphasis would need to be given to identification of priority, research, funding, leading to technological transfers. These aspects would take into account full cognizance of environmental, social and financial impacts. This would be achievable through increased interaction between inter-industrial sectors, industry and academia, industry and government, taking into account inputs from the UN Agencies and other active role players, such as IUPAC.

As is now the case in Japan, there needs to be an appreciation of integration of the environment and business.

In countries in transition pragmatic implementation of environmental legislation was a problem requiring expert input. This was achievable as industry in such countries adopted the principle of Responsible Care, the needs for improvements in cost accounting and many of the other aspects of Green Chemistry discussed during this symposium.

Mervyn L. Richardson
BASIC, Birch Drive, Rickmansworth, Herts, WD3 2UL, UK

Fate and effects of contaminants in soils as influenced by natural organic material

This article summarizes the essentials of a symposium held at the Fraunhofer-Institute for Environmental Chemistry and Ecotoxicology 16–18 September 1996 under the auspices of IUPAC, the Commission on Water and Soil Chemistry and the Gesellschaft Deutscher Chemiker, Fachgruppe für Umweltchemie und Ökotoxikologie.

In recent years processes of interactions between contaminants and physical as well as chemical soil parameters have been intensively studied to achieve advances in the hazard and risk assessment of contaminants in soils. As regards soil organic matter major research areas have been sorption and binding processes. A more recent area includes the influences of natural organic matter (NOM) and the dissolved part (DOM) on mobility, bioavailability and toxic effects of heavy metals and organic contaminants.

The role of dissolved natural organic compounds in the field has been identified to be a major one both with respect to the analytical facet of the problem as well as regards modifications in fate and effects of contaminants.

Formation and characterization of soil organic matter

Depending on the use of the soils (e.g. forest, pasture, agriculture) the amount, composition and properties of the litter and plant residues (roots and leaves) are the dominant factors for humification in the terrestrial environment. Since soil organisms, especially the microbial biomass (the micro-organisms themselves and their excreta) play an important part in the carbon cycle, they are also involved in the humification processes.

From a physical chemical point of view, the formation of soil organic matter proceeds as:

- the formation of particulate organic matter originating from larger sized parts of the litter resulting in stabilized organic matter particles of high binding capacities like lignite but with a slow migration of pollutants into their inner pore system;
- humification of natural high and low molecular substances and coating of soil mineral particles by this organic material; and
- formation of dissolved organic matter in the soil solution.

The soil organic matter in layers below the A-horizon should be taken into consideration especially concerning the behaviour of organic contaminants in soil. The long-term behaviour of soil organic matter is another important topic. In this context only information on the classical differentiation of soil organic matter into fulvic and humic acids and insoluble humins is routinely available. More information is needed for the classification of organic matter with respect to its stability and binding and mobilization processes of pollutants.

New concepts and their modelling require the distinction of soil organic matter in its functions within the carbon-cycle in soil. Upon the decay processes the plant residues will lead to structure carbon, metabolic carbon, active carbon, slow degradative soil carbon and passive soil carbon. From a scientific point of view the characterization of solid soil organic matter also includes the differentiation of the soil particle sizes since it influences OM quantity and quality.

Separation of agricultural top soils according to their particle sizes resulted in more than 40% of the organic matter in the clay fraction demonstrating that soil particles are coated during the formation of the insoluble organic matter. The particulate and dissolved humic substances are refractory due to the structure of the organic matter and due to the building of organic-mineral complexes.

For the classification and characterization of organic matter different highly sophisticated methods are available or under development. One recently often used technique is NMR spectroscopy to elucidate the chemical composition of humic substances with respect to carboxylic carbon, aromatic carbon, o-alkyl carbon and alkyl carbon. Pyrolysis-GC/MS and pyrolysis-GC/AED are methods aiming for the analysis of building blocks of isolated organic matter, enabling polymers of natural and anthropogenic origin to be distinguished. The information content on building blocks and their binding state in the organic matter backbone can be enhanced by thermally-assisted hydrolysis and methylation. FTIR and ^{1}H-NMR spectroscopy are used for recognizing origin, building blocks and degree of humification of organic matter.

The splitting-off of functional groups and the breakdown of the polymer network upon organic matter degradation can be traced effectively by TG-MS and TG-FTIR. The pyrolysis-MS studies performed with organic matter at both atmospheric pressure and high vacuum (insource mode) indicate a high proportion of pyrolysis residues (about 40 wt%) upon heating to 750 °C. The released pyrolysis products include mainly

nonspecific, low molecular-weight compounds which are at present of limited value for characterizing the polymeric network. The TG-FTIR coupling turned out to be only useful in recognizing low molecular compounds such as H_2O, CO_2, CO, H_2S, COS, CH_4 and NH_3 which show distinctive absorbance patterns. The use of these techniques for OM characterization thus is still open.

Regarding residue analysis in soils, soil organic matter has not only an important influence on amount and quality of non-extractable residues in soils but also on the kind and amount of clean-up procedures required prior to analysis. The recovery of contaminants depends on the quantity and quality of the solid soil organic matter and on the quantity and quality of the dissolved organic matter in soil solution. An influence of the soil pH is also given. If the co-extracted organic matter is not carefully removed it will interfere with proper separation and quantification of pollutants. On the other hand these clean up steps may lead to a substantial loss of the pollutants. Especially the content of dissolved organic matter should be taken into consideration when interpreting analytical results of environmental samples.

Interactions of contaminants with SOM

Affinity capillary electrophoresis (ACE) has been used to investigate the binding processes between s-triazines and soil as well as water extracted fulvic and humic acids (FA and HA). The distribution coefficients of the s-triazines between the dissolved humic substances and the water phase were found to be a function of the degree of ionisation of both s-triazines and ligands, indicating both ionic and hydrogen bonding types of interactions. Furthermore, micellar electrokinetic chromatography (MEKC) experiments showed that the interactions of the s-triazines with HA could be described as a partitioning of the s-triazines between water and the dissolved organic humic phase. Similar to surfactants, humic acids behaved like ionic micelles in the aqueous buffer at concentrations higher than a defined 'humic critical micellar concentration' (HCMC). The low molecular weight acidic fulvic acids (FA) behaved the same way but showing higher HCMC. These results confirm the micellar properties of HS and the hydrophobic type of interaction of the s-triazines with hydrophobic sites of humic and fulvic ionic micelles.

The use of solid phase microextraction (SPME) in combination with headspace-GC/MS or GC/AED techniques was applied to investigate the sorption process of polycyclic aromatic hydrocarbons (PAH), polychlorinated biphenyls (PCB), chlorinated pesticides and tin organic compounds to humic organic matter (HOM). These techniques were used to investigate the sorption kinetics and to determine partition coefficients (K_{OC}). The results showed that hydrophobic, nonpolar interactions dominate the sorption process of PAH, PCB and chlorinated pesticides to HOM. However further experiments have to elucidate whether HOM coats the fibres to an extent that will change the sorption properties and kinetics.

Stationary and time-resolved laser-induced fluorescence (LIF) and fluorescence quenching studies were used for the investigation of humic substances (HS) and their interactions with polycyclic aromatic compounds (PAC). Aqueous solutions of HS of different origin (e.g. aquatic, soil or peat HS) were investigated with these techniques both with and without the presence of PAC. The fluorescence quenching efficiencies, expressed by the Stern-Volmer constants (K_{SV}), depend on the fluorophor (PAC) as well as on the HS. From the temperature and pH dependencies of the K_{SV}-values, information on structural variations of HS and on the thermodynamics of PAC/HS interactions was obtained. The suitability of these sophisticated techniques was demonstrated in soil column experiments, but has to be further improved.

Desorption kinetics vary considerably dependent on the experimental procedure used, e.g. column experiments may lead to different results compared to flask-shaking experiments. Time-resolved column leaching procedures provide information useful for the understanding of the organic matter to pollutant interaction. They allow to distinguish between spontaneous desorption and a subsequent diffusion controlled steady-state. The extent of both processes is closely related with each other. The desorption kinetics and amounts are significantly dependent on the composition of the eluent. In general, the stronger eluents (e.g. $Na_2H_2PO_4$) provoke distinct desorption peaks, indicating a strong alteration of the organic phase by the eluent, while the elution profile of weak eluents (e.g. $CaCl_2$) are quasi-constant and appear, thus, to be governed by slow diffusion processes from inner spheres of the particulate matter towards the surface.

However, column studies have the disadvantage that they are difficult to standardise with respect to flow rate, desorption solution and homogeneity of the soils (homogeneous water flow through the soil column is essential).

The dependence of the association between a sparingly soluble organic contaminant and DOM can also be shown by batch techniques. Results confirm that the sorption of contaminants strongly depends on:

- the origin and composition of the organic matter;
- the physico-chemical characteristics of the pollutants; and
- the solute chemistry (e.g. pH-value, salt content and composition (ionic strength).

The origin of humic matter and its sorption properties also influence the sorption of organic substances to

sewage sludges. It was shown that the sorption capacity as related to the organic carbon content of the sewage sludges is comparable to that of agricultural top soils. This example demonstrates that appropriate and simple methods are needed which can be routinely used for a characterization of the dissolved and particulate organic matter with respect to their sorption potential.

Enhancement of mobility by dissolved organic matter

Measurements of PAH-concentrations in different soil horizons show the migration of the hardly soluble PAHs from the topsoils of a high organic matter content to subsoils. This migration can only be explained by a co-transport with DOM. Model experiments with DOM fractions from composts show that the binding capacity of high molecular DOM fractions is significantly higher than those of low molecular fractions. Nevertheless DOM fractions of a molecular size below 1000 D showed also interactions with PAHs. For the DOM fractions two types of interactions can be postulated. Sorption of hydrophobic substances on hydrophobic regions within the macromolecules and interactions of the substances with hydrophobic sites and amphoteric low molecular weight DOM molecules. The solubilizing effect is correlated with the hydrophobicity of the substances, with the sorption to the soil matrix and it also depends on the composition and origin of the DOM and the overall chemical composition of the solution. As regards the importance of the origin of DOM it could be shown that fungal metabolic products significantly enhance the solubility of hydrophobic organic chemicals.

For an assessment of ground water pollution which may be caused by a mobilization of hardly soluble toxic substances sorption and desorption processes in the three phase system soil–DOM–water, the properties of the DOM and its sorption to soils need to be considered. Mathematical models are under development to simulate these processes. First results show that:

- a three-phase model provides satisfying simulation results.
- an *a priori* prediction of HOC mobility based on the three-phase partition models is possible.
- the identification of relevant processes is impossible with 'classical' experimental designs.
- inverse modeling might result in misinterpretation of experimental data sets.
- nonlinearity is an important fact in HOC sorption.

Numerical simulations confirm the observations, that DOM influenced mobility of HOC in porous media is

- increased due to co-transport.
- reduced due to co-sorption and/or cumulative sorption, and;
- controlled by site-specific physicochemical properties.

Effects of natural organic matter on the fate of substances

Binding of xenobiotics to humic matter influences their degradation in soil. Führ *et al.* investigated the effect of straw amendment on the formation and translocation of residues of ^{14}C-methabenzthiazuron with laboratory and lysimeter experiments. The lysimeter experiments performed with an orthic luvisol (pH 7.2; 1.2% OC; 6.4% sand; 78.2% silt; 15.4% clay) showed that the amendment of straw to the plough layer according to agricultural practice resulted in a significant increase of the degradation and mineralization of methabenzthiazuron but also in the formation of bound residues. In the fraction of bound residues larger amounts of radiocarbon were found in fulvic and humic acids compared to the radioactivity in humines. The enhancement of microbial activity, mineralization and degradation rate were comparable to laboratory experiments. Increasing amendment with straw material resulted in an even more rapid formation of bound residues. Additionally, the amount of methabenzthiazuron in the leachate was affected. Although the amount of leachate was the same in the lysimeters with and without straw amendment, the total amount of transferred methabenzthiazuron was considerably lower in the lysimeter with straw amendment.

Upon addition of wheat straw, lucerne leaves and farmyard manure in experiments with ^{14}C-labelled isoproturon different ratios between dissolved organic carbon and dissolved radioactive material as well as different metabolite patterns in percolates of small-scale column experiments were observed. The amount of bound residues increased with time and differed dependent on soil treatment. Generally, the quality and not the quantity of the added organic matter was decisive for the results in these experiments.

The binding behaviour and the nature of binding of the fungicide anilazine and the herbicide amitrole to dissolved organic matter was investigated by Spiteller *et al.* Using ^{13}C-NMR-spectroscopy one type of linkage of anilazine to humic matter was characterized as a covalent ether-bonding in soil, compost and lake water. This was underlined by experimental breaking the bond using TMSCl and the identification of the corresponding trimethylsilylether-derivate. A postulated covalent linkage of amitrole to humic matter was also investigated and confirmed by ^{15}N-NMR-spectroscopy. However, besides covalent binding also hydrogen-bonding and/or charge-transfer complexes have to be considered. In the case of amitrole an inhibitory effect on plant growth was observed due to remobilized amitrole, identified in DMF/TMSCl-extracts of the incubated plants.

Bioavailability and ecotoxicity

The ecotoxicological potential of a soil is determined by investigation of soil organisms (terrestrial ecotox-tests) or as a substitute with limited evidence by the use of aquatic ecotox-tests for example with daphnids, algae, luminescent bacteria using soil extracts.

To achieve realistic interpretation of each ecotox-test its limitations have to be taken into account. Tests with soil organisms give information about the habitat function of a soil. With aquatic ecotox-tests toxic bioavailable contaminants are determined. Contaminants are detected which can be eluted from the soil. Therefore information on the retention function of the soil and on possible contamination of groundwater are obtained. There is general agreement that for an intensive assessment of a soil the different exposure paths of the investigated organisms have to be considered.

Soil organisms—The results of several studies with earthworms indicate that soil organic matter content has an important influence on the accumulation and toxicity of a range of chemicals (metals and non-polar compounds). However, the availability and hence the effects of these two groups of chemicals are additionally modified by other co-variable factors. For metals, e.g. soil pH plays a major role for free metal ion concentrations in the soil pore water, while for non-polar compounds the lipophilicity of the compound is the most important co-determining factor. As organic matter reduces the uptake and the toxic effects of a range of pollutants by organisms it can be concluded that the maintenance of high levels of organic material in contaminated soils is important.

The uptake and transfer of plant available heavy metals from soil into plants furthermore depends on plant specific factors based on genetic differences with respect to the properties of the root system, selectivity against different metals, inner plant translocation mechanisms, transpiration rate etc. Last but not least the general growing conditions (climatic conditions, nutrient supply, duration of the vegetation period) also influence the heavy metal transfer from soil into plants. The evaluation of several experiments elucidates that generally SOM has a relatively low influence on the uptake of heavy metals by plants. The direction of this influence is still controversially discussed. May be that a further differentiation of SOM as shown for example by Kögel-Knabner *et al.* is necessary to show any clear dependency of parts of the SOM on the transfer of heavy metals from soil into plants. Even if relationships between parts (fractions) of the SOM and the uptake of heavy metals by plants will be elaborated it will be difficult to put this knowledge into administrative rules. For practical purpose the use of neutral salt extractions is the best solution because the different influences of soil specific parameters can be sufficiently considered. Furthermore NOM seems to influence the biomass weight

Problems with Ecotoxicological Tests / Outdoor/Field Investigations

Test System	Advantage	Potential Disadvantages/Problems
acute aquatic tests	• quantification of the toxicity via dilution series	• preparation of eluates • correction of pH-value? • at least partially low sensitivity (only high concentrations can be detected) • coloring of the extract • Interference of the test systems/organisms with micro-organisms, which had been extracted • fairly soluble substances cannot be detected
chronic aquatic tests (algae test)	• quantification of the toxicity via dilution series	• see acute aquatic tests • nutritional problems
terrestrial tests (added organisms)	• (in)direct statements/conclusions in regard of habitat functions • different exposure pathways can be determined to a certain extent	• uncontaminated control often not available, consequently dilution series cannot be carried out • ⇒ only severe impacts are detectable (plant test) • due to the chemical-physical and pedologic conditions the habitat may not be optimal for the test organisms
terrestrial investigations (soil endogenous organisms)	• direct statement in regard of habitat functions • determination of different exposure pathways	• uncontaminated control often not available, consequently dilution series cannot be carried out • ⇒ only severe impacts are detectable • abundances/activities for important organisms must be determined depending on soil substrates and land use (so far very few data are available)

of roots and shoots. Both inhibition and stimulation have been observed, presumably depending on plant species.

Tests with aquatic organisms—When using aquatic tests with soil extracts a precise measurement of the dissolved contaminants or exclusion of particles is necessary. Design of the tests and the chemical exposure analyses should provide for the definite distinction between aquatic and particulate exposure, in order to avoid totally misleading results with soil extracts.

Specific and conclusive experiments investigating the influence of DOM on toxicity of chemicals have been so far mainly performed with aquatic organisms. Depending on experimental design not only enhancement of toxicity (phototoxicity) but also masking of toxicity were observed. In one experiment, e.g. the daphnia, toxicity of lindane and pendimethalin could be reduced to 'not measurable' upon addition of natural DOM.

Conclusion

Available evidence clearly shows a significant influence of dissolved organic matter in soils and waters on the fate and effects of chemicals. This role of natural organic carbon in environmental compartments is in addition and partly directly contrary to the conventional role which has been thoroughly investigated and considered in legislation. In order to quantify and elucidate the significance of dissolved organic matter in the real environment with respect to risk assessment of contaminants, systematic, well-targeted investigations are needed.

W. Kördel
Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, D-57392 Schmallenberg, Germany

Dedicated to Prof. Werner Klein on the occasion of his 60th birthday

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most recent list of the national/regional centres appeared in *Chemistry International* 1995, **17**, 141.

Names for Inorganic Radicals

Radicals are important in a variety of catalytic processes and in the atmospheric gas and liquid phases; furthermore a substantial number of inorganic radicals have been observed in interstellar gas clouds.

In biology, the interest in radicals increased after the discoveries that superoxide and nitrogen monoxide are formed *in vivo*; these radicals play an important role in cell–cell signalling, the immune response and disease.

Rules have been developed to name inorganic radicals in a systematic manner.

It was found that for inorganic radicals coordination nomenclature yielded unique names that are descriptive of composition and structure (where known).

The strategy to name a radical is to select a central atom and name all other atoms (or groups of atoms) as ligands, or, if the name ends in '-yl' and the Ewens–Bassett number. As an example, CO_2- is named 'dioxidocarbonate-yl(1-)'.

These rules are intended to replace those found in Section I-8.4 of *Nomenclature of Inorganic Chemistry, Recommendations 1990*, Blackwell Scientific Publications, Oxford, 1990 (the 'Red Book').

Comments on these recommendations are welcome and should be sent by 30 November 1997 to: Prof W.H. Koppenol, Laboratorium für Anorganische Chemie, Eidgenössiche Techniche Hochschule, Universitätstrasse 6, CH-8092 Zürich, Switzerland. Tel.: +41 1 632 2875; Fax: +41 1 632 1090; E-mail: koppenol@inorg.chem.ethz.ch

Recommendations for the presentation of NMR structures of proteins and nucleic acids

During the past several years the determination of NMR solution structures of small proteins has found widespread application, and the NMR method is being used increasingly for structural studies of nucleic acids and their complexes with proteins, drugs and other molecules. In the course of this development, a certain con-

sensus has developed on the presentation of NMR solution structures. This has been helped indirectly by guidelines established for depositing primary experimental data and resulting structures in databanks such as the Protein Data Bank, BioMagResBank, Nucleic Acid Database, and by conventions used for abstracting services, for example, *Macromolecular Structures*, Current Biology, London, UK, 1991ff. In consideration of making good future use of the experience accumulated during the past few years, the present Task Group has been convened as an IUPAC/IUBMB/IUPAB Inter-Union venture, which was also supported by ICSU and CODATA. The group has gone through formal examinations of the reporting conventions of biomolecular NMR used in the past. The present recommendations also build upon earlier rules for biochemical nomenclature and for the presentation of proton and non-proton NMR data. Consultation with a large fraction of the leading research groups in the field of NMR structure determination with biological macromolecules indicates that these guidelines will be widely accepted by the community.

Comments on these recommendations are welcome and should be sent by 30 November 1997 to: Prof. Kurt Wüthrich, Institut für Molekularbiologie und Biophysik, ETH-Hönggerberg HPM, CH-8093 Zürich, Switzerland. Tel.: +41 1 633 24 73; Fax: +41 1 633 11 51; E-mail: wuethrich@mol.biol.ethz.ch

Comments

The work of IUPAC has featured recently on the 'Editor's Page' of both *Chemistry in Britain*, published by the Royal Society of Chemistry, UK, and *Chemical & Engineering News*, published by the American Chemical Society. The two articles are reproduced below.

An editor's lot is not always a happy one...

...observes Richard Stevenson, Editor of *Chemistry in Britain* and Chairman of the Association of British Science Writers.

'What's in a name? That which we call a rose, by any other name would smell as sweet.' And certainly brimstone smells as pungent whether it is called sulphur or sulfur—but try telling that to some chemists. A number of eagle-eyed readers noted that last month's *Chemistry in Britain* carried the cover line 'Chemistry of sulfur'. Innocent enough in all conscience, but a hanging offence according to one correspondent, who wrote: 'I look to the Royal Society of Chemistry to uphold standards in our subject and feel that you have failed to do this'.

Yet when IUPAC (in 1990) and the RSC (in 1992) adopted 'sulfur' as the correct spelling for element 16, *Chemistry in Britain* hung back—only to be told off by other correspondents, one of whom wrote: 'We try to persuade students that they must abandon old habits and move with the times...our efforts are not aided when they open their *Chemistry in Britain*'.

Readers who are interested enough can look up the correspondence we published at the time (*Chem. Br.*, April 1992, p. 324; July 1992, p. 604), but suffice it to say that I promulgated the doctrine that *Chemistry in Britain*, being aimed at a wider audience than the RSC's primary and secondary journals, would continue to use the familiar 'sulphur', at least until general usage began to reflect the change.

However, last year I was persuaded by the *Chemistry in Britain* Editorial Board to relax this ruling, so that dyed-in-the-wool sulfur chemists could spell their element that way if they so wished. This is not the only case where *Chemistry in Britain* allows two forms of nomenclature to run in parallel. For example, the nomenclature rules adopted by the Association of Science Education mandate the use of 'ethene' and 'ethyne', which would be unrecognisable to their industrial colleagues used to making and selling ethylene and acetylene. Even IUPAC accepts these two trivial names. Being pragmatic, *Chemistry in Britain* accepts whichever an author prefers, though leaning towards the spellings familiar to our predominantly industrial readership.

Industry, of course, can be slow to move: an academic acquaintance tells the story of visiting—not all that many years ago—a petrochemical plant and asking what the labels 'OV' and 'MA' meant on two of the site's pipelines. 'Oil of vitriol and muriatic acid', he was told. A former colleague—who as a subeditor had been a punctilious user of the education world's 'ethene' and 'ethyne'—joined that same petrochemical company as a press officer. A few weeks into the job she telephoned me on the QT to ask what 'muriatic acid' was, because she didn't want to appear stupid. Humphry Davy identified and named chlorine as far back as 1810, yet the fertiliser industry does still sometimes refer to 'muriates'

not chlorides.

One argument for rigid nomenclature is that searches on computers with massive memories but very little intelligence will not pick up references to sulfur if you key in sulphur. Yet I recently saw a scientific paper on 'diatom–diatom interactions' and had to read a lot further before I could be sure the authors meant reactions between H_2 molecules and not relations between little silica-walled algae in ponds. What is a dumb computer to make of that?

The 'ultras' of chemical nomenclature will not have it, of course. Off with decadent Sulphur's head! Etymologically correct Citizen Sulfur is to take over the kingdom. My pragmatism in allowing dual standards will see me reviled by both sides, while my comrades in the ranks of scientific editors (for whom House Style Rules OK!) will have me cashiered and my red pen broken before my eyes.

I am still waiting for my US colleagues to face up to IUPAC's ruling that 'aluminum' and 'cesium' are wrong.

Reprinted from Chemistry in Britain *(May 1997) with the permission of its Editor.*

The antiscience cancer

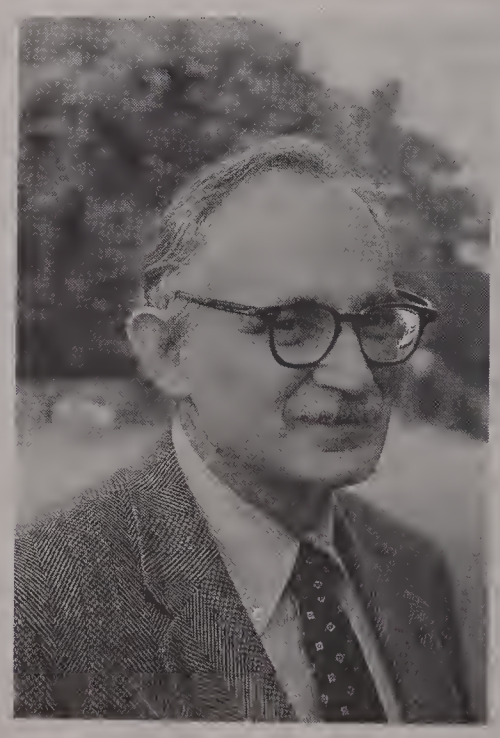
A guest editorial by Allen J. Bard, Norman Hackerman-Welch Regents Chair in Chemistry at the University of Texas, Austin, Editor of the *Journal of the American Chemical Society* and President of IUPAC during 1991–1993.

In February, NBC televised a movie called 'Terminal' about a physician who had discovered the cure for a particular form of cancer. Rather than revel in his discovery, he sought out wealthy patients who were in the hospital for other ailments, surreptitiously infected them with this form of cancer (which he apparently could induce to appear in days like a bad cold) and then came to their rescue with his cure. These patients were so grateful that they showered him with funds to support his research. Even more scurrilous than this far-fetched story, however, were the postmortem comments shown with the credits. These claimed that scientists were competing for the monetary rewards that will come with the discovery of a cure for cancer and that 'so far they have only discovered how to cause cancer'.

The antiscience flavor of this movie is only one example of the attack on science in the US from all sides. From the left, the postmodernists declare that science does not really deal with facts and that accepted models only represent the opinion of the scientific establishment. Those with a particular social agenda rewrite the history of science and create scenarios that have little connection with reality and actual science. For example, the notorious 'Baseline Essay on Science' adopted by the Portland, Ore., Public Schools seeks to promote multiculturalism by proposing fantastic contributions of ancient inhabitants of Africa (*Phi Delta Kappan*, November 1993, p. 266). These include knowledge about the moons of Jupiter, acquired in pre-telescope days through parapsychological powers. This essay also proposes that melamin can convert light to knowledge and also absorb the wave energy of magnetism. On the right, creationists want to teach religious concepts as science. On other fronts, a large fraction of the populace believes in ghosts, angels, ESP, astrology, and magic crystals.

Scientists usually respond to such attacks and anti-intellectualism from a defensive posture. We try to explain the fallacies in the arguments and hope that better education will undo the attackers. This approach has not worked very well in the past, and it will be a disaster to wait the length of time it would take to produce an educated populace to deal with these immediate problems. Seventy years after the Scopes trial and the widespread teaching of evolution, school districts still are under attack by fundamentalists, and a law punishing teachers of evolution came close to passing in late March in the Tennessee legislature.

It is time for scientific societies to take the offensive and attack the pseudoscience and misinformation eating away at our profession. For example, they could establish offices and member networks to respond quickly to antiscience attacks and to aid groups fighting creationism and pseudoscience in their school districts. If the TV movie had the equivalent racial or sexual overtones, NBC would have been inundated with letters and protests, supported by a number of organizations. Yet we sit by and passively watch and hope that people will recognize the fantasy in the presentation.



Prof. Allen J. Bard

Scientists also should confront the sociologists and philosophers at their institutions who are attacking the foundations of science. Presumably, tenure decisions and promotions at universities are based on scholarship, and academic scientists must take an interest in the academic decisions in other departments on campus. This is not a question of academic freedom, but rather one of competency. We should expose political correctness and fundamentalism that lead to misinformation about science.

We also should clean our own house and speak out when scientists overplay their findings or promise more than they can deliver. We must be totally honest when discussing the impact of our work in real world situations and in differentiating unsupported opinion from conclusions drawn from sound research. Shoddy work and bad science should be exposed. However, if the mainstream scientific organizations, like ACS, the American Association for the Advancement of Science, the National Academy of Sciences, the Council on Chemical Research, and the International Union on Pure and Applied Chemistry just sit back and watch, the future of science, at least in the US, is bleak indeed.

Reprinted from Chemical & Engineering News *(22 April 1996) with the permission of the American Chemical Society.*

Letter to the Editor

In the November 1996 issue of *Chemistry International,* Dr John Duffus of Heriot-Watt University, Scotland, challenged the previous publication (*Chemistry International*, May 1996) of a figure showing the toxicity of various chemical elements taken from the set of teaching aids, DIDAC-1, produced by Agfa-Gevaert. Two members of the DIDAC working group at Agfa-Gevaert who were co-responsible for the contents as well as the illustrations of the teaching aids respond:

(1) The aim of Prof. P. De Bièvre's article in *Chemistry International* 1996, **18**(3), 96, was to report about the initiative taken by the Belgian National Committee for Chemistry to celebrate IUPAC's 75 years, coinciding incidentally with the 100th anniversary of Agfa-Gevaert N.V.

(2) As a present to the Belgian teachers of chemistry a package of teaching aids for chemistry containing 63 full-colour transparencies, a black-and-white copy of each transparency for easy photocopying and distribution to pupils and an accompanying explanatory text available in Dutch, French or English was made available to every participating teacher. Prof. P. De Bièvre mentioned this in his report. The IUPAC secretariat, at its own initiative, selected a transparency from the series and added it to the article of Prof. P. De Bièvre as an illustration, of course without the accompanying explanatory text available to the teacher.

(3) No doubt, the comments of Dr J. Duffus on the illustrative transparency as such (the black-and-white version) are correct. Unfortunately, the text accompanying the transparency is missing: '...it can be demonstrated that certain elements which are listed as harmful or toxic, are also essential for the metabolism of living beings. In this apparent contradiction lies the answer to the question: when is a chemical substance harmful or dangerous? It all depends on the type and degree of exposure to the substance and the amount absorbed by the living organism. Danger is a relative concept.' Moreover the published transparency is to be used in conjunction with another related transparency, demonstrating the abundance of the elements in living organisms.

Thus it can be concluded that the comments of Dr. Duffus and the explanatory text in DIDAC-1 present the same ideas.

In the meantime we are pleased to let you know that DIDAC already contains three volumes and that the volumes 4, 5 and 6 are in preparation. The working group is composed of about 20 high-level research people of Agfa-Gevaert and authorities of our five Flemish universities, whose aim is to make chemistry lessons attractive to young people in order to stimulate further learning and simultaneously eliminating the often misunderstood image and role chemistry has.

Yours sincerely,

Jan De Roeck & Eddy Michiels,
Agfa-Gevaert N.V.,
On behalf of the working group DIDAC

New Publications

Kemisk Ordbog

A Danish handbook of IUPAC nomenclature has been authored by the Nomenclature Committee of the Danish Chemical Society. Dr Ture Damhus, Principal Scientist at Novo Nordisk A/S, Member of the Nomenclature Committee, writes:

Just before Christmas 1996, a book was published in Denmark which aims to become the source of IUPAC nomenclature rules for everyone interested in expressing chemistry and chemistry related matters in a consistent way in Danish.

The Nomenclature Committee of the Danish Chemical Society was revitalized a few years ago and took on the responsibility for providing a comprehensive reference document for chemical nomenclature in Danish, something which had not really existed before. The basic idea was to translate loyally the newest IUPAC rules so that, in principle, the only thing we would have to do was to change the names of elements and parent compounds into their Danish counterparts.

The task was not entirely trivial, however. The *spelling* of chemical names has been the subject of heated debate in Denmark, on and off, since the days of the late Prof. K.A. Jensen (known in IUPAC circles from his period as Chairman of the Commission on Nomenclature of Inorganic Chemistry and for his broad interest in all chemical nomenclature issues and in linguistic matters in general). Prof. Jensen argued that the spelling in Danish should be as close to international (i.e. English) spelling as possible whenever the chemical names were the same, whereas his opponents—including *Dansk Sprognaevn,* an official body given the authority to decide on correct spelling in Danish in general—insisted on a traditional Danish spelling. Examples under debate included: calcium/kalcium; chlor/klor (for chlorine); chrom/krom (for chromium); ether/aeter; iod/jod (for iodine); methyl/metyl; phosphor/fosfor (for phosphorus); phenol/fenol; quinin/kinin (for quinine). Also, certain elements had special Danish names.

Interestingly, when starting our work on Kemisk Ordbog, we found that, in practice, the debate about the spelling and choice of element names had been resolved quietly by two very influential sectors of the chemical community. One, Danish gymnasium (high school) teachers had decided on the international spelling when writing completely new series of textbooks in connection with a restructuring of the school system around 1990—textbooks that were not likely to be replaced for many years. The other area where a clear stand had already been taken in the 1980s, with the spelling debate still raging, was in administration dealing with environmental and occupational health and safety laws, i.e. laws regulating the use of chemicals and thus encompassing extensive lists of names of chemical substances.

With official laws and educational text books formulated with international spelling, it was quite clear that we also should go for this choice in the new nomenclature book, and so we did.

It must be said that there were other problems unrelated to internal Danish quarrels. Merging the recommendations of all the available IUPAC nomenclature sources, as we endeavoured to do, is not easy, e.g. prescriptions in the Red Book and the Macromolecular Nomenclature compendium are in a number of cases at variance with those found in the Blue Guide (partly due, of course, to the different publication dates of these various recommendations). Hopefully, we have found reasonable compromises and judged correctly what will become the future IUPAC names in cases of present inconsistency.

Kemisk Ordbog starts with a list of almost 10 000 names of individual chemical compounds and names of structurally defined classes of compounds. The explanations for these entries are corresponding 'Danish IUPAC names' and definitions of the class names in terms of structure, respectively. Trivial names and obsolete spellings and names are included as entries, but the reader is, in principle, always directed from these to IUPAC names.

The second part of the book consists of text chapters dealing with the IUPAC nomenclature rules and also with related subjects such as etymology and principles for constructing INN (International Non-proprietary Names) for drugs.

The third part of the book consists of a number of tables in the spirit of the tables in the Red Book and the Blue Guide, giving the element names, multiplicative prefixes, collections of parent hydride structures, lists of substituent group names and so on.

Nomenklatura Chromatograficzna

A Polish edition of Nomenclature for Chromatography recommended by IUPAC [*Pure Appl. Chem.* 1993, **65**(4), 819] has been prepared by the Commission of Chromatographic Analysis of the Committee of Analytical Chemistry of the Polish Academy of Sciences.

***Nomenklatura Chromatograficzna**, edited by Zygfryda Witkiewicza, Edwarda Soczewinskiego & Zdzislawa Suprynowicza, is published by Polski Narodowy Komitet, Warsaw 1996, ISBN 83 901844 4 3.*

World Health Organization Publications—Environment

This catalogue provides bibliographic and descriptive information for some 50 WHO publications concerned with the ways in which protection of the environment can promote human health. Publications are grouped according to the following topics: environmental analysis; environmental health promotion; environmental policy; water supply, sanitation; wastewater; air quality; ultraviolet radiation; natural disasters; nuclear power; hazardous wastes; vector control; urbanization; radiation protection; the WHO Environmental Health Criteria series.

Several of these books describe national and international policies intended to protect the environment and the human life it sustains. Others consolidate world knowledge on the best technologies for meeting the fundamental need for safe water and safe methods of waste disposal—whether involving garbage collection in urban slums or the 'recycling' of precious water resources. Still others establish environmental standards that can guide efforts to monitor pollution, ascertain the safety of air and water, or protect against exposure to hazardous chemicals and pesticides. In line with WHO policy, the catalogue also features several practical training guides that can help communities understand the links between environmental conditions and health - and take appropriate action.

***World Health Organization Publications—Environment,** March 1997, is available from WHO Distribution and Sales, 1211 Geneva 27, Switzerland. Fax: +41 22 791 4857.*

Conferences

International Symposium on Calorimetry and Chemical Thermodynamics, Universidade Estadual de Campinas, Campinas, SP, Brazil, 5–9 April 1998

IUPAC
SPONSORED

This conference, sponsored by IUPAC and the Instituto de Quimica, Universidade Estadual de Campinas, will focus on the recent advances in the field of calorimetry and its application to studies dealing with chemical and biological systems. Other approaches to the determination and discussion of thermodynamic aspects in such systems are also welcome. It aims to be a truly international conference, with the participation of the experts in these fields, and is also intended to be an opportunity for Latin American scientists of these areas, especially younger ones, to meet their colleagues from other parts of the world.

The scientific programme is based on four sessions, dealing with basic and applied aspects of the following subjects: biological systems (living and non-living), solutions (reactive and non-reactive systems), solids and interfacial systems, applied thermodynamics (with special emphasis on biotechnology) and other related topics. A workshop on 'Molecular and Reaction Energetics' organized by Prof. J.A. Martinho Simões, Portugal, will also be part of the programme.

The meeting schedule will include plenary lectures, invited lectures, oral presentations and a poster session.

There is a proposal for organizing an electronic version of this Symposium (a Virtual Conference). It would allow the submission of complete versions of the oral and poster presentations which would be accessible and open for discussion during a certain period. Participation is voluntary and open for those who did not attend the Symposium. Its realisation will depend on the responses to the First Circular.

The registration fee is USD 200 before 1 December 1997, USD 250 after 1 December 1997, for scientific participants, and USD 100 before 1 December 1997, USD 120 after 1 December 1997, for students/young scientists. This fee includes the conference material, morning and afternoon coffee/tea, a cocktail reception, a Brazilian barbecue and daily transportation between the hotels and the conference centre.

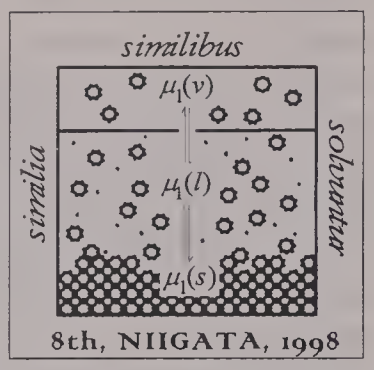
For further information, please contact: Dr. Watson Loh, Instituto de Quimica - UNICAMP, Caixa Postal 6154, 13083-970 - Campinas - SP - Brazil. Tel.: +55 19 239 7881; Fax: +55 19 239 3805; E-mail: wloh@iqm.unicamp.br

More information about the conference, its location and tours is available at the conference Home Page (http://www.iqm.unicamp.br/~wloh/conf). This information will be routinely updated.

8th International Symposium on Solubility Phenomena, Niigata, Japan, 5–8 August 1998

IUPAC
SPONSORED

This international symposium, sponsored by IUPAC and the Japan Society for Analytical Chemistry, will be concerned with many aspects of solubility phenomena and related areas of chemistry. The scientific programme includes plenary and invited lectures, oral communications and poster presentations in the following fields:



1 Chemistry of crystallization and dissolution.
2 Analytical chemistry related to phase transfer.
3 Thermodynamics and kinetics in solution.
4 Biomineralization.
5 Solubility phenomena of pollutants and environmental chemistry.
6 Compilation and evaluation of solubility data.

The registration fee is ¥ 35 000 before 15 March 1998, ¥ 45 000 after 15 March 1998, for scientific participants, and ¥ 10 000 before 15 March 1998, ¥ 15 000 after 15 March 1998, for students.

A second circular, with call for papers, registration and accommodation forms, will be mailed in the autumn of 1997.

To receive the second circular, please contact: Kiyoshi Sawada, General Secretary of the 8th ISSP, Department of Chemistry, Faculty of Science, Niigata University, Niigata 950-21, Japan. Tel.: +81 25 262 6265; Fax: +81 25 262 6116; E-mail: issp@sc.niigata-u.ac.jp

Conference Calendar

1997

Ionic polymerization

7–11 July
International Symposium on Ionic Polymerization. Paris, France.
Symposium Secretariat, Chantal Iannarelli, Congrès Scientifiques Services, 2 Rue des Villarmains, F-92210 Saint-Cloud, France. Tel.:+33 (1) 47 71 90 04. Fax: +33 (1) 47 71 90 05.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic. Tel.: +42 (2) 360341; Fax: +42 (2) 367891; E-mail: sympo@imc.cas.cz

Vacuum microbalance techniques

16–18 July
27th International Conference on Vacuum Microbalance Techniques. Lublin, Poland.
Dr P. Staszczuk, Department of Physical Chemistry, Faculty of Chemistry, Marie Curie-Sklodowska University, M. Curie-Sklodowska Sq. 3, 20-031 Lublin, Poland. Tel.: +48 (81) 5375646/+48 (81) 5375784; Fax: +48 (81) 5333348; E-mail: piotr@hermes.umcs.lublin.pl/ rdobrow@hermes.umcs.lublin.pl

Organometallic chemistry

20–25 July
9th International Symposium on Organometallic Chemistry Directed Towards Organic Synthesis. Göttingen, Germany.
Prof. A. de Meijere, Chairman OMCOS 9, Institut für Organische Chemie, Georg-August-Universität Göttingen, Tammannstrasse 2, D-37077 Göttingen, Germany. Tel.: +49 (551) 39 32 32; Fax: +49 (551) 39 9475; E-mail: ucoc@uni-goettingen.de

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules, Surface and Interfacial Phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic. Tel.: +42 (2) 360341; Fax: +42 (2) 367891; E-mail: sympo@imc.cas.cz

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of

Chemistry & Biotechnology, Graduate School of Engineering, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan. Tel.:+81 (3) 38122111 ext. 7261; Fax: +81 (3) 58006945

Medicinal chemistry

29 July–1 August
AIMECS'97: AFMC International Medicinal Chemistry Symposium. Seoul, Korea.
Dr H. Park, Secretary General, AIMECS 97, c/o The Korean Chemical Society, #703, The Korean Science & Technology Center, 635-4, Yeogsam-Dong, Kangnam-Gu, Seoul 135-703, Korea. Tel.: +82 (2) 34534019; Fax: +82 (2) 5696673; E-mail: hpark@kistmail.kist.re.kr

Interfaces against pollution

10–13 August
International Conference on Interfaces Against Pollution. Wageningen, Netherlands.
IAP97, PO Box 8038, 6700 EK Wageningen, Netherlands. Tel.: +31 (317) 482279; Fax: +31 (317) 483777; E-mail: iap97@fenk.wau.nl

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* **14**, 203 (1992).

Plasma chemistry

18–22 August
13th International Symposium on Plasma Chemistry. Beijing, China.
Dr Lin He, Chinese Society of Theoretical & Applied Mechanics, 15 Zhong Guan Cun Road, Beijing 100080, China

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
AKM Congress Service, PO Box 37, CH-1218 Le Grand-Saconnex/GE, Switzerland. Tel.: +41 (22) 7611661. Fax: +41 (22) 7611662

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion

Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile.
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (2) 6811644; Fax: +56 (2) 6812108; E-mail: jcostama@lauca.usach.cl

Polymers

25–28 August
12th Bratislava Conference on Polymers: Modified Polyolefins for Advanced Polymeric Materials. Bratislava, Slovak Republic.
12th Bratislava International Conference on Polymers, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta 9, 842 36 Bratislava, Slovak Republic. Tel.: +42 (7) 3782198. Fax: +42 (7) 375923. E-mail: upolebor@savba.sk

Solution chemistry

26–31 August
24th International Conference on Solution Chemistry, Centre Omnisport, Vichy, France.
Prof. P. Turq, Laboratoire d'Electrochimie, Université Pierre & Marie Curie, Case courier 51, 4 place Jussieu, 75252 Paris Cedex 05, France

Electron transfer processes

3–7 September
International Symposium on Electron Transfer Processes and Reactive Intermediates in Macromolecular and Organic Chemistry. Zabre, Poland.
Prof. Z.J. Jedlinski, Institute of Polymer Chemistry, Polish Academy of Sciences, ul. Marii Curie Sklodowskiej 34, 41-800 Zabrze, Poland. Tel.: +48 (32) 1716077; Fax: +48 (32) 1712969; E-mail: polymer@usctoux1.cto.us.edu.pl

Colloquium spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997. Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel.: +61 (3) 98193700; Fax: +61 (3) 98195978.

Emulsions

23–26 September
2nd World Congress on Emulsions: Industrial Applications of Emulsions. Bordeaux, France.
Mr A. Le Coroller, Directeur-Général, CME, 50 place Marcel Pagnol, 92100 Boulogne-Billancourt, France. Tel.: +33 (1) 47617689; Fax: +33 (1) 47617465 .

Green chemistry

28–30 September
International Conference on Green Chemistry: Challenging Perspectives. Venice, Italy.
Conference Secretariat, Green Chemistry: Challenging Perspectives, Consorzio Interuniversitario Nazionale 'La Chimica per l'Ambiente', Facolta di Scienze Matematische, Fisiche e Naturali, Calle Larga S Marta 21.37, 30123 Venezia, Italy.

Macromolecule–metal complexes

6–10 October
7th International Symposium on Macromolecule-Metal Complexes (MMC-7). Noorwijkerhout, Netherlands.
Prof. J. Reedijk, Leiden Institute of Chemistry, PO Box 9502, 2300 RA Leiden, Netherlands. Tel.: +31 (71) 5274459. Fax: +31 (71) 5274451; E-mail: reedijk@rulgca.leidenuniv.nl

Biodiversity and bioresources

23–27 November
International Conference on Biodiversity and Bioresources—Conservation and Utilization. Phuket, Thailand.
IUPAC Biodiversity Conference, National Center for Genetic Engineering and Biotechnology, National Science and Technology Development Agency Building, 73/1 Rama VI Road, Bangkok 10400, Thailand. Tel.: +66 (2) 6448150-4, ext. 505, 532, 534; Fax: +66 (2) 6448107-8; E-mail: iupacconf@biotec.or.th

1998

Polymer sciences and technology

5–10 January
International Symposium on Advances of Polymer Sciences and Technology. Madras, India.
Dr K.S.V. Srinivasan, Deputy Director & Head, Polymer Division, Central Leather Institute, Council of Scientific & Industrial Research, Adyer, Madras - 600 020, India.

Calorimetry and chemical thermodynamics

5–9 April
International Conference on Calorimetry and Chemical Thermodynamics. Campinas, Brazil.
Prof. C. Airoldi, Instituto de Química, UNICAMP - CP 6154, Universidade Estradul de Campinas, 13081-970 Campinas sp, Brazil.
http://www.iqm.unicamp.br/wloh/conf/

Trace element speciation

4–7 May
1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences. Neuherberg, Munich, Germany.
First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, FRG. Tel.: +49 (89) 31873030 (2669); Fax: +49 (89) 31873362.

Degradation processes in the environment

24–28 May
International Conference on Degradation Processes in the Environment. Dubrovnik, Croatia.
Dr A. Sabljic, Institute Boskovic, POB 1016, HR-10011 Zagreb, Croatia

Organic synthesis

28 June–2 July
12th International Conference on Organic Synthesis. Venice, Italy.
Depha Congress SRL, Viale Majno 21, 20122 Milano, Italy. Tel.: +39 (2) 76008190; Fax: +39 (2) 782400; E-mail: dephadue@mbox.vol.it

Chemistry in Africa

6–10 July
7th International Chemistry Conference in Africa (7th ICCA). Durban, South Africa.
The Secretary, 7th ICC & 34th SACI Convention, Department of Chemistry & Applied Chemistry, University of Natal, Durban 4041, South Africa. Tel.: +27 (31) 3603090. Fax: +27 (31) 2603091; E-mail: 7icca@che.und.ac.za

Macromolecules

20–23 July
18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.
P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, CZ-162 06 Prague 6, Czech Republic.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all *bona fide* chemists from throughout the world to attend irrespective of race, religion, or political philosophy. IUPAC sponsorship implies that entry visas will be granted to all *bona fide* chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

Tel.: +420 (2) 360341; Fax: +420 (2) 367981;
E-mail: sympo@imc.cas.cz

Chemical thermodynamics

26 July–1 August
15th International Conference on Chemical Thermodynamics. Porto, Portugal.
Prof. M.A.V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal.

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (171) 4378656; Fax: +44 (171) 7341227.

Novel aromatic compounds

2–7 August
9th International Symposium on Novel Aromatic Compounds, Hong Kong.
Prof. H.N.C. Wong, Chairman, Local Organizing Committe, 9th International Symposium on Novel Aromatic Compounds, Department of Chemistry, Chinese University of Hong Kong, Shatin, New Territories, Hong Kong.

Solubility phenomena

5–8 August
8th International Symposium on Solubility Phenomena. Niigata, Japan.
Prof. H. Akaiwa, Faculty of Engineering, Gunma University, Kiryu 376, Japan.

Physical organic chemistry

16–21 August
14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.
Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento di Química, 88040-900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy. Tel.: +39 (55) 2757549. Fax: +39 (55) 2757555.

Medicinal chemistry

6–10 September
25th International Symposium on Medicinal Chemistry. Edinburgh, Scotland.
Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (0)171 437 8656; Fax: +44 (0)171 734 1227.

Natural products

11–16 October
21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.
Prof. Xibai Qiu, Secretariat of ISCNP-21, c/o Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: +86 (10) 62568157 or 62564020; Fax: +86 (10) 62568157; E-mail: qiuxb@infoc.3.icas.ac.cn

2000

Macromolecules

9–14 July
MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.
Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90-363 Lodz, Poland. Tel.: +48 (42) 819815; Fax: +48 (42) 847126.

Biotechnology

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.

b
Blackwell Science

Osney Mead,
Oxford OX2 0EL,
UK

Telephone
(01865) 206206

Fax
(01865) 206096

Pure and Applied Chemistry

IUPAC

Official Journal of the International Union of Pure and Applied Chemistry

Since 1960 the Union has made available to chemists everywhere a very large amount of important material which it handles each year through its regular publication in Pure and Applied Chemistry. The objectives of the journal are:

- to publish the main invited lectures of symposia sponsored by IUPAC at which authoritative and up-to-date accounts of the subject of the symposium are presented by prominent scientists; the lecturers cover their own recent work and review the worldwide literature on the subject;
- to publish the recommendations of the Union's commissions on nomenclature, symbols and units;
- to publish technical reports on standardization, recommended procedures, collaborative studies, data compilations, etc.;
- to publish critically evaluated state-of-the-art commissioned review articles on important topics.

Subscription Information

Pure and Applied Chemistry is published monthly. Subscription rates for 1997 are for institutions are £672.00 (Europe), £736.00 (overseas) and US$1020.00 (USA & Canada). Individual subscription prices for 1997 are £82.00 (Europe), £82.00 (overseas) and US$115.00 (USA & Canada).

Order Form

Please tick the appropriate box and return to Karen Edge at the address opposite:

☐ Please enter my 1997 Institutional subscription to *Pure and Applied Chemistry*

☐ Please enter my 1997 Individual subscription to *Pure and Applied Chmistry*

☐ I wish to pay by cheque and enclose the sum of £_____ US$_____

☐ I wish to pay by Access/American Express/Diners Card/VISA/Mastercard/JCB

(delete as necessary)

Please debit my credit card no. | | | | | | | | | | | | | | | | |

Expiry date _____ with the sum of £_____ US$_____

Signature _____ Date _____

European Community VAT & Canadian GST

Subscribers in Europe must quote their VAT registration number or state that they are not VAT-registered. Subscribers in the following countries who are not VAT-registered must add VAT to the subscription price at the appropriate rate: Belgium (6% TVA/BTW); France (2.1% TVA); Germany (7% MwSt); Spain (4% IVA); The Netherlands (6% BTW).

All subscribers in Canada must add 7% to allow for GST.

☐ Please send me a specimen copy of *Pure and Applied Chemistry*

Name _____

Address _____

_____

http://www.blackwell-science.com

International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

President: A. E. FISCHLI (*Switzerland*)
Vice-President: J. JORTNER (*Israel*)

Secretary-General: E. D. BECKER (*USA*)
Treasurer: J. M. WARD (*UK*)

IUPAC Secretariat

Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK.
Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 39 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Neue Schweizerisches Chemische Gesellschaft **(Switzerland)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1997, Vol. 19, No. 4 (July)

95 Secretary General's Column
Edwin D. Becker

96 39th IUPAC General Assembly

104 Report of the International Union of Pure and Applied Chemistry: 1996
Mo Williams

108 IUPAC Accounts for 1996
J.W. Ward

113 News

119 Safety Evaluation of Pesticide Residues in Food

127 Conference Reports

140 Provisional Recommendations

141 Comments

143 Letter to the Editor

144 New Publications

145 Conferences

146 Conference Calendar

Information on this magazine can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

b
Blackwell Science

0193-6484(199707)19:4;1-W

Printed in Great Britain by Alden, Oxford, Didcot & Northampton

ISSN 0193-6484

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

1997, Vol. 19, No. 5 (September)

Blackwell Science

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

PRODUCTION EDITOR: Howard Waller

All correspondence to be addressed to The Editor, Chemistry International, IUPAC Secretariat, PO Box 13757, Research Triangle Park, NC 27709-3757, USA. Telephone: +1 (919) 485 8700. Fax: +1 (919) 485 8706. E-mail: johnwjost@compuserve.com and http://chemistry.rsc.org/rsc/iupac.htm

Editorial Advisory Board

Chairman:	E. D. BECKER	*Secretary General*
	E. BUNCEL	*CHEMRAWN Committee*
	A. SMITH	*Committee on Chemistry and Industry*
	D. H. M. BOWEN	*Committee on Printed and Electronic Publications*
	I. M. MILLS	*Interdivisional Committee on Nomenclature and Symbols*
	M. E. PESTANA	*Committee on Teaching of Chemistry*
Acting Secretary:	J.W. JOST	*Executive Director*

G. SOMSEN	*Division I*
G. J. LEIGH	*Division II*
G. SAVELLI	*Division III*
A. ABE	*Division IV*
F. INGMAN	*Division V*
T. R. ROBERTS	*Division VI*
(To be appointed)	*Division VII*

Subscriptions

Six issues of *Chemistry International* will be published bimonthly in 1997 (one volume per annum) in January, March, May, July, September and November. The 1997 subscription rate including postage is GBP 75.00 (UK and overseas except North America) or USD 116.00 (US and Canada). The individual subscription rate is GBP 29.00 (UK and overseas except North America) or USD 42.00 (US and Canada). Microfiche subscriptions are available simultaneously with the printed edition, and microfilm at the end of the subscription year. Subscription orders may be placed directly with IUPAC's official publisher, Blackwell Science Ltd, PO Box 88, Oxford, UK; E-mail: journals.cs@blacksci.co.uk. Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Advertising. Enquiries should be sent to the Advertising Manager, Blackwell Science Ltd, Osney Mead, Oxford OX2 0EL, UK. Telephone: +44 (0) 1865 206206, Telex 83355 Medbok G, Fax +44 (0)1865 721205.

Despatch. The news magazine is despatched within Europe by surface mail, to other continents by various forms of air-speeded delivery: to the US* by air freight for forwarding by periodicals post, to India by air freight for guaranteeed local delivery, and to all other countries by Accelerated Surface Post.

Reproduction of Articles

Unless there is a footnote to the contrary, reproduction or translation of articles in this issue is encouraged, provided that it is accompanied by a reference to the original in *Chemistry International*. The Blackwell Science logo is a trade mark of Blackwell Science Ltd registered at the United Kingdom Trade Marks Registry.
This journal is included in the ADONIS service, whereby copies of individual articles can be printed out from compact discs (CD-ROM) on demand.

*Periodicals postage paid at Rahway, NJ. Post Master, send address changes to *Chemistry International*, c/o Mercury Airfreight International Inc., 2323 Randolf Avenue, Avenel, NJ 07001, USA.

Front cover: The former First National Bank, Philadelphia, now home of the Chemical Heritage Foundation (see page 161).

International Union of Pure and Applied Chemistry

Relocation of the IUPAC Secretariat

From 30 September 1997, all correspondence should be directed to the office of the new Executive Director:

Dr John W. Jost
IUPAC Secretariat
PO Box 13757
Research Triangle Park
NC 27709-3757
USA

Tel.: +1 (919) 485 8700
Fax: +1 (919) 485 8706
E-mail: johnwjost@compuserve.com

During October the Oxford Secretariat will be occupied in shipping files to RTP and to the Chemical Heritage Foundation in Philadelphia (see page 161) and in disposal of furniture and equipment.

The President's Report

Albert E. Fischli

It has been a very busy presidency up to now and I am convinced that it will remain so until the end of the year. In these days of rapid globalization, we can readily perceive the effects that the high-speed changes taking place around us are having on IUPAC. Yet globalization is not new to IUPAC: looking back over the Union's history, we see that globalization was an important topic as early as 1919 and that it was the driving force behind the creation of IUPAC just after the First World War. Globally accepted standards, codices and nomenclature for chemicals had the same prime importance for academia and industry then as they have now. This being said, however, I have to add that IUPAC's objectives, as set out in our Statutes, give the Union a much broader mandate.

Today, the rapid pace of growth and change in the basic experimental sciences of biology, chemistry and physics is apparent to all. Looking at the information explosion in these areas, our attention is frequently drawn to the crossover between the sciences and to the fact that Nature is—alas—not organized like our universities. Adaptation and flexibility are needed in academia as well as industry.

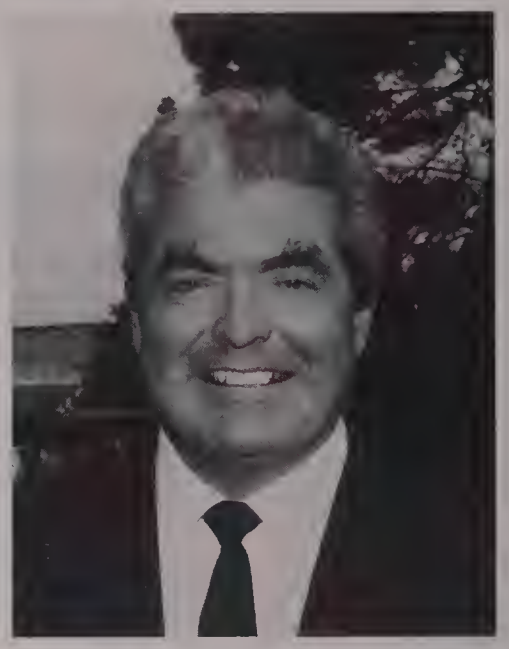
Moreover, it is our responsibility as scientists to ensure that both government and the public at large are made aware of scientific progress at an early stage. In particular, our task as chemists is to put over the message that chemistry is already very important today and that it will go on to be a key science in the world of tomorrow, with a tremendous outreach into sister sciences, the environment, industry and the economy as well as into our everyday lives.

Achievements

Administration and finances

As you are aware, Dr Mo Williams, who was head of the IUPAC Secretariat from 1968, retired this year at the end of April. You will also be aware that our new Executive Director, Dr John W. Jost, took up his post at Research Triangle Park (RTP), NC, USA, at the beginning of April. The transitional period, during which there will be two Secretariats, will last until September 1997. In October our Oxford office will ship documents to RTP and then close down.

At this point in my report I feel privileged to have the opportunity to express my sincere thanks to Mo Williams for his long and outstanding service, and for his loyalty during his time with IUPAC. He personified stability for a substantial part of IUPAC's existence and



was also the leading authority on all matters relating to IUPAC. At the same time I also want to extend my very best wishes to our new Executive Director, who is building up our new USA Secretariat into a globally active Secretariat, devoting special care to emphasizing activities which will ultimately enhance IUPAC's visibility.

As part of this process, our web site (current Home Page address http://chemistry.rsc.org/rsc/iupac.htm) will be further enlarged and made more accessible by setting up a main site at RTP with the domain name of iupac.org. The current site, hosted by the Royal Society of Chemistry, will become our European mirror site. We expect soon thereafter to have also an Asia/Pacific mirror site. It is intended that the site should become the chief channel of communication with the community and especially with those engaged on IUPAC projects.

Our finances are now in good shape, thanks to the work of our Treasurer, as well as to the Finance Committee and the new USA banker taking care of our securities. These have been supplemented by windfall money from Barings Bank. The Executive Committee decided that the Treasurer should set up a new endowment fund to harbour our surprise resources.

Congresses

I would like to pick out just three of the many IUPAC-sponsored conferences that have taken place or are still to take place this biennium.

This year, for the first time since 1967, the IUPAC Congress and General Assembly (GA) have been scheduled to take place in the same city in two successive weeks—'back to back', so to speak. The venue is Geneva, Switzerland, and the two events will be taking

place in the last two weeks of August; the Congress first, then the GA. The same pattern will be repeated in 1999 in Berlin, Germany, after which IUPAC will be able to take proper stock of the new combined event. Holding the two events in successive weeks obviously increases the organizing committees' workload substantially, and I would like to express my thanks to the two organizing bodies in Switzerland and Germany who have taken up the challenge.

In fall 1996 the CHEMRAWN IX Conference took place in Seoul, Republic of Korea, under the heading 'The Role of Advanced Materials in Sustainable Development: Use, Disposal and Recycling of Materials'. Thanks above all to a magnificent effort by the South Korean industry, the event was a great success. Incidentally, this was the third time that IUPAC has had the pleasure of holding a CHEMRAWN Conference in the Asian/West Pacific Rim region: the other two were 'Chemistry and World Food Supplies' in Manila in 1982 and 'Advanced Materials' in Tokyo in 1987.

A third IUPAC workshop on Safety in Chemical Production was organized in April 1997 by our industrial wing COCI, the Committee on Chemistry and Industry. The workshop was held in San Francisco, CA, in conjunction with the American Chemical Society, the US Chemical Manufacturers Association and the US Environmental Protection Agency. The attendance of two 1995 chemistry Nobel laureates generated keen interest. After the first workshop, which was held in Basle, Switzerland (1990), and the second, which was held in Yokohama, Japan (1993), there is still continued interest in holding workshops in other parts of the world.

Nomenclature

I am happy that IUPAC is now able to submit a final list of names and symbols for elements 101–109 to the Council for approval in Geneva in August this year. As you are aware, the naming of the transfermium elements was a lengthy, controversy-ridden process. The three laboratories in Germany, Russia and USA which were involved in the discovery of the elements have been consulted at length and their comments solicited. Their input was most important, given that one of IUPAC's responsibilities is to formulate widely accepted recommendations capable of forming a basis for international communication in chemistry. A press release was issued in February 1997 and the final say rests with the Council. I should also mention that activities have been started to enable IUPAC to put forward proposals for the nomenclature of elements 110–112. The process will be conducted in accordance with our Bylaws and in close collaboration with the discoverers. Once these activities have concluded the final decision will once again be made by the IUPAC Council.

Collaboration with UN and ICSU Bodies

Collaborative efforts with UNESCO, UNIDO and WHO have been substantially intensified during the biennium.

CHEMRAWN IX was organized jointly by our CHEMRAWN Committee and UNESCO, while COCI continued its three-way collaboration with UNIDO and UNESCO. This gives safety experts from the Third World the opportunity to spend a period of approximately one month with IUPAC Company Associates and discuss existing safety measures in a direct hands-on fashion. The visiting safety experts, a substantial number of whom were government specialists, subsequently returned to their home countries. We are thus constructing a progressively expanding network of safety experts in chemical production and also bringing IUPAC into closer contact with the developing world.

All the programmes which IUPAC is undertaking in conjunction with UNESCO are supervised by the International Chemistry Council (ICC), a body comprising four chemistry Nobel laureates from Canada, France, UK and USA, one Japanese industrialist and three developing world representatives from Africa, Asia/Pacific and Latin America. The inaugural meeting took place in Paris in January 1997. The executive part of the programmes is in the hands of IUPAC and UNESCO Officers. The ICC will convene every second year to make a critical assessment of all joint IUPAC/UNESCO activities. We will also be inviting representatives of our Committee on Teaching for Chemistry (CTC) to take part in IUPAC's annual meetings with UNESCO. This is because CTC has been collaborating with UNESCO for quite some time in areas of key interest to the ICC. Furthermore, some of our Commissions have been enlisting UNESCO's help to have larger-scale programmes followed up. Such joint activity also presents an opportunity for us to strengthen our links with the International Organization for Chemical Sciences in Development (IOCD) and the Third World Academy of Sciences (TWAS).

The President of our Division on Chemistry and the Environment is acting as WHO liaison. He is representing our interests at the WHO-led International Forum for Chemical Safety (IFCS) and International Programme for Chemical Safety (IPCS). In the course of his duties, he will be maintaining very close contact with the President of our Division on Chemistry and Human Health. IUPAC together with IUPHAR, IUTOX and the International Life Science Institute (ILSI) constitute the scientific ICSU-NGOs in these UN bodies. IUPAC is currently acting as the group's spokesman.

Collaboration with ICSU executive bodies, a large number of sister unions, ILSI and the ICSU Scientific Committee on Problems of the Environment (SCOPE) has improved substantially in 1996–97.

Chemistry and society

In October 1996 COCI published its first White Book as a contribution from science to the debate on the effects of chlorine and chlorine-containing compounds on the environment. This 'White Book on Chlorine', published as a special issue of the IUPAC journal *Pure and Applied Chemistry*, is an independent and unbiased collection of original articles written by renowned scientists from all over the world, which critically evaluates various aspects of the subject. It has proven to be a success and of interest not only to academic institutions, industry, governmental agencies and environmental organizations, but also to the general public.

The White Book is the first publication of this type and more are set to follow. IUPAC is thus able to use its special position as a science-based, non-governmental, non-industry foundation with a world-wide network of experts from various fields of chemistry and sister disciplines to offer a platform for publications.

State of the Union

Countries and companies

A glance at the world map of National Adhering Organizations (NAOs) and Observer Countries (OCs) shows that while IUPAC is represented in all but a few areas of the Americas, the West Pacific Rim and Europe, it has as yet failed to enlist broad participation from either the strip of countries stretching from Syria to Kazakhstan or the countries of Africa—with the exception of Egypt, the Republic of South Africa and Tunisia. Egypt and South Africa have both been affiliated to IUPAC for quite some time now. This year the Executive Committee will have the pleasure of submitting to the Council in Geneva the membership application of the Union of Yugoslav Chemical Societies as well as requests for upgrading from Pakistan and the Philippines, two of our Observer Countries. Let me add at this juncture that our well accepted voting system is special in that it reflects the countries' actual chemical turnover figures as published by the UN. As a rule, while NAOs with stronger chemical and pharmaceutical industries have a somewhat larger voting share in the Council, they also make a greater financial contribution to IUPAC.

The participation of single companies—IUPAC is the only scientific union with direct industry participation—is remarkable, and membership of the Company Associate scheme remains astonishingly stable given the conditions which industry has to contend with today. Top of the participating companies table in 1996 was Japan with 46 companies, followed by USA with 23 and Germany with 12. The EU15 have 44 altogether. Comparing financial contributions for 1996, USA is on first place, followed by Japan and Germany. The EU15 are on second place behind USA.

Adapting mission, goals and structures

My predecessors' State of the Union reports discussed the critical remarks voiced against some of IUPAC's activities in considerable depth. Incidentally, some of these criticisms are still the subject of discussion. I would like here to inform you about the actions taken in 1996–97 in response to valuable constructive criticism. I believe that the steps we have taken will result in goals and structures which reflect the tasks facing IUPAC in the next millennium.

Several brainstorming sessions took place during the biennium at which IUPAC Officers, all of whom were very much involved in the organization of the meetings, were able to discuss thoroughly IUPAC's current situation, mission, objectives and future. These always involved well-known chemists from academia and industry, plus representatives from inside and outside IUPAC. An initial meeting was held in Belmont, USA, during June 1996. A subsequent European one-day meeting was organized in London for February 1997 and a third brainstorming workshop for the Asia/Pacific region took place in Singapore during June 1997. All were very fruitful in clarifying IUPAC's mission and goals as it heads into the next millennium as well as in promoting an intensive and rewarding exchange of opinions about the strengths and weaknesses of the Union. The meetings reinforced the need for the changes being discussed in IUPAC. All were extremely valuable, instrumental even, in the formulation of new objectives and activities, and to increasing IUPAC's visibility.

The IUPAC Officers also held an extraordinary meeting with the Divisional Presidents/Vice-Presidents and Section Presidents in Frankfurt, Germany, in March this year. This meeting was an opportunity to go through each Division's restructuring plans. While the creation of the Divisions on Chemistry and the Environment and on Chemistry and Human Health at the last General Assembly represents a major step there are still some desiderata. We need to find ways of integrating both the area of materials and the major scientific activities taking place at the interface between chemistry and biology into IUPAC. With the Divisional Presidents' input, the Frankfurt meeting yielded proposals for solutions which should result in structural changes to eliminate overlap and provide IUPAC with the missing activities and structures. The meeting was also used for a thorough discussion of the Vice-President's Critical Assessment and to some extent for discussion of further proposals for structural change.

These proposals and the Vice-President's Critical Assessment were taken up again at the Executive Committee (EC) meeting at Jerusalem in April 1997. After detailed discussions the EC decided to establish a Strategy Development and Implementation Committee

(SDIC) to define the science policy of the Union and to examine the feasibility of converting the bulk of IUPAC's scientific work to a project-driven/project-financed system with time-limited Commissions, as described in the concept endorsed by the EC. The eleven members of the SDIC were appointed by myself following consultations. The Committee was placed under the chairmanship of Vice-President Joshua Jortner and it met for the first time in June.

Scientific work

I am delighted at the large number of committed volunteers who devote their time and scientific expertise to furthering the IUPAC cause. More than 1000 scientists are actively involved in IUPAC, an achievement which I strongly believe to be cause for congratulation. That this is an enormous strength goes without saying, and we have to safeguard its continuity under the best possible circumstances. It also goes without saying that the limited financial resources available to IUPAC and the small time window available for new scientific endeavours are forcing us to choose our projects carefully.

Future perspectives

As the only purely scientific global chemical organization mandated to undertake this kind of work, it is essential that IUPAC continues with its codification, nomenclature and standardization activities. It has to do so at a much faster pace than in the past and in close association with the professional bodies which are also involved in these activities. They are working rapidly using their excellent skills, and IUPAC should try to find a collaborative basis with them which is not only acceptable to all stakeholders, but which will also enable all parties to benefit from the special advantage which IUPAC derives from being a global, strictly scientific, non-governmental organization.

It is also my belief that collaboration with UN and ICSU bodies has to be intensified and focused. Here IUPAC has a special responsibility, arising from the immense outreach of chemistry into the other sciences and the remarkably close relationship which has existed for quite a long time between chemistry in academia and the now giant chemical and pharmaceutical industry. This relationship has no parallel in physics and has started to emerge in biology only relatively recently with the advent of small biotechnology companies, the first of which was set up in California in 1976. Chemistry is a pervasive part of our everyday lives and one that accompanies us throughout our lives.

For these reasons, IUPAC should also increase its activities in the field of 'Chemistry and Society'. Here again the Union occupies a very special position, maintaining as it does close contact with all the major stakeholders in innovation, i.e. academia, industry, government and society. We have been successful in strengthening our links with society, and through society with governments as well; nevertheless, I think, there is still a lot of room for improvement.

As always, there are still some issues to be resolved. One is that all of us in IUPAC have to make greater efforts to recruit the best scientists for our activities. This is extremely important to IUPAC since all our collaborators are volunteers. One of the advisors whom I had the pleasure of consulting during my period as Vice-President summed it up by saying that serving IUPAC comes under the heading of *noblesse oblige*.

A second unresolved issue is that we have to be very careful in selecting the activities in which we wish to get involved. We have to make sure that we are resolute in the pursuit of our goals once they are defined and that we come up with the desired result quickly. Let me also add that we have to remain true to our scientific base, unswayed by any pressure of a non-scientific nature, irrespective of whether it comes from academia, industry, governments or society.

Conclusions

Significant progress has been made, but a lot still remains to be done.

I have enjoyed having responsibility for a large number of teams, and I feel privileged to have been able to work with such colleagues as my fellow IUPAC Officers and the Members of the Secretariat, Executive Committee and Bureau as well as to have interacted with the Council, IUPAC's highest body. I am also very pleased to have been given the opportunity to establish contacts with our Divisional Presidents as well as with the Chairmen of CHEMRAWN, COCI, CTC, the Committee for Printed and Electronic Publications (CPEP) and the Committee on Affiliate Membership (CAM). If we look at CAM, it becomes apparent that, although progress has been made, there is still a need for further action. Additionally, CPEP is in need of a new policy on the submission of papers for publication in *Pure and Applied Chemistry*.

Let me close by thanking all members of IUPAC bodies for their efforts and the dedication with which they have worked for our Union over the last biennium in particular, even though I am aware that most of them have been working on IUPAC's behalf for substantially longer. It is due to them, their commitment, flexibility and creativity, that we can look with confidence to the future of IUPAC.

Secretary General's Report

Edwin D. Becker

The IUPAC Statutes give the Secretary General the responsibility for carrying out the business of the Union, keeping its records and administering the Secretariat. There are many aspects of the organization and management of our operations that fall into these categories and that are currently the subject of intense analysis and discussion. Since reports on those activities will largely be included in the presentations by other Officers, I would like to concentrate here primarily on the Secretariat, which is one of the most visible physical manifestations of the Union and which plays a central role in the smooth functioning of IUPAC.

Since the last Council meeting two years ago, there have been major changes in the Secretariat, as you know. Let me review briefly the reasons for those changes, then describe the current status and plans for the new Secretariat in Research Triangle Park, North Carolina, USA (RTP).

Location of the Secretariat. IUPAC first established an independent permanent Secretariat headed by a full time professional staff member in 1968. Since that time the Secretariat has been located in Oxford, UK, under the direction of Dr Maurice (Mo) Williams. Two years ago, when I was elected Secretary General at Guildford, I was well aware of the fact that Mo was scheduled to retire in April 1997, that two other long-time senior staff members had recently retired or were slated to retire by 1998, that the fourth professional staff member was potentially interested in other opportunities, and that one of the supporting secretarial staff would also retire in 1998. I also soon became aware of on-going discussions on possible relocation of the Secretariat; certainly this concatenation of personnel loss suggested that this was an appropriate time to consider such a move. Initially I was opposed to a move. With the awesome responsibility for recruiting several new staff members, I was concerned (as were a number of others) that the disruption of a move would be more than IUPAC (and I as Secretary General) could handle. However, over the next few months I completely changed my views, and ultimately the Executive Committee overwhelmingly came to the conclusion that a move to RTP was desirable. There were three factors that influenced me, and I think, the Executive Committee:

- Prof. Albert Fischli (then Vice-President) convincingly articulated the view that IUPAC, as a global organization, should think globally in terms of all its activities, including future locations of the Secretariat. He pointed out that with modern electronic communications, the Secretariat could be located almost anywhere, yet be in instant contact with activities in all countries. In keeping with the pace of modern international research and the activities of multinational companies, he advocated that a move of the Secretariat every 10 years or so should be considered to enhance IUPAC's global image.

- As I analysed the activities in the Secretariat and put new information together with my long experience as a Commission Chairman and as Chairman of the Committee on Publications, I became convinced that we could and should introduce major changes in the scope, organization and conduct of the Secretariat's activities. While these could probably be accomplished in Oxford, where we would have the benefit of the experience and dedication of several talented staff members who would remain, there would inevitably be compromises in trying to adapt new methods to an existing organization. I also became convinced that, with careful management and the cooperation of the staff in Oxford, a transition to a new location could be effected without the 'absolute chaos' that some had predicted. (So far, this expectation has proved valid, and I am confident that when the move is completed later this year, we will continue to feel only moderate moving pains.)
- We received three offers of rent-free space: in Paris, Frankfurt and RTP. The first two were very attractive, and we are grateful for the generosity of the Maison de la Chemie and Gesellschaft Deutscher Chemiker for inviting IUPAC and for offering assistance beyond the well appointed space. Either would have placed the Secretariat in the centre of a bustling metropolis, with many cultural advantages, but with the significant disadvantage of the high salaries and other costs associated with such cities. RTP, on the other hand, is well outside the high costs of downtown New York, Washington and other cities;

salaries, fringe benefits and living costs there are generally well below those of Frankfurt and Paris. RTP is, however, the centre of a major research hub, with 38 000 people employed in research and light manufacturing in the Research Park itself (which includes research laboratories of several major multinational pharmaceutical and electronics companies). RTP is located at the centre of a triangle formed by three major universities—Duke, University of North Carolina and North Carolina State University—and there are many formal and informal scientific and technical interchanges among the organizations in the RTP area. The advantages of this site proved irresistible.

At RTP we have a 10-year, rent-free lease on a 4000 square foot prefabricated building, provided by the Research Triangle Foundation (RTF), a non-profit organization that serves as the developer of the Research Park. Not only has the RTF furnished the building, but they voluntarily spent over USD 20 000 to redecorate the interior of the building for our use. Since the building provides more than enough space for our near-term needs, we have subleased a portion of the building for five years to the *Journal of Endocrinology* for its editorial office, thus bringing in income that should largely offset utility and other related costs.

A New Executive Director. Recruiting a successor for Mo Williams presented the next challenge. Not only would we lose Mo's expertise, but we also would lose several long-time dedicated staff members and their collective knowledge of the Union. While many of Mo's talents are irreplaceable, we felt that we had an opportunity to recruit an individual with a suitable background and abilities to lead the Secretariat into its next era.

We advertised widely and received about 70 applications from 10 countries. I am very pleased that Dr John Jost has joined us as Executive Director. After conducting research in basic physical chemistry and spectroscopy, Dr Jost spent 22 years with Unocal (a major international oil company) in research management and administration. He has brought to IUPAC a rich mix of managerial talent, hands-on experience in information technology and wide experience in chemistry.

John has begun to organize the office in RTP, while we continue the Oxford office until the end of September. This arrangement has permitted him to continue routine activities with the Oxford staff while he analyses the operations and prepares to recruit at RTP only the staff essential to the projected modes of operation.

Basic Functions of the Secretariat. In addition to the essential functions of the Secretariat related to financial management, record-keeping and general administration, the areas viewed as especially important for the new Secretariat are those relating to communications with IUPAC volunteers, Affiliates and the world-wide chemistry community. This emphasis on communication makes the Union's electronic communication and publishing activities a central activity of the Secretariat. It is expected that by fall a new site for the IUPAC Home Page will be established in North Carolina with its own domain name. In addition to retaining the current site at the UK Royal Society of Chemistry as a mirror site, we expect to attract other mirror sites in the Asia/Pacific region and Eastern Europe. The Home Page will be developed into a central communication and publication hub for the Union.

Under guidelines developed last year by our Committee on Printed and Electronic Publications (CPEP), preliminary Commission Reports will be disseminated mainly electronically rather than as paper. The electronic version made available for comment will, of course, be clearly identified as preliminary. The electronic format will allow the submission of comments easily and quickly. It is expected that publication of preliminary documents in this fashion will greatly increase the visibility of IUPAC Commission Reports in the chemical community.

In addition, CPEP currently has under review other specific proposals to publish final Commission Reports and Conference Proceedings electronically in conjunction with usual publication in *Pure and Applied Chemistry*. There are also on-going discussions of improvements in the print version of *Chemistry International* with ancillary electronic communications on the IUPAC Home Page. It is planned to begin making *CI* available on the Internet in parallel with the print edition late in 1997 or early in 1998. This should make the content of *CI* more widely available than it is currently and enable it to function better as a method of promoting feedback from the chemical community outside the circle of those directly involved in Union activities.

New Support Role for the Secretariat. With economies brought about by relying on information technology, we should require fewer staff members to carry out strictly administrative activities and can recruit professional staff who will be able to give more attention to the needs of our Commissions in carrying out their projects. As part of the concept adopted by the Executive Committee to emphasize a project-driven structure, we will need a better system to help Commissions develop proposals, recruit candidates to serve on Commissions, track projects and provide progress reports. With the full support of the Executive Committee, John Jost is moving carefully to ensure that our routine administration is being handled well, while he determines the staffing needs for implementing this new role. We believe that in the next two years you will see a dramatically transformed Secretariat, which will be able to provide the kind of support that our Commissions need to initiate, carry out and complete important projects in a timely way and to obtain rapid publication of their reports.

Biennial Report of the Treasurer and Finance Committee

J.M. Ward

As I did for the last Council Meeting, I shall give a report of the first year of the present biennium and one of the previous complete biennium 1994–95. I shall also attempt to estimate the outcome for the present year. Also, as this is my last year as Treasurer, I think I should give you a brief summary of my stewardship during the last six years.

I give below the amounts transferred to the Balance Sheet from the Expenses and Income Accounts, i.e. the 'bottom lines' and the corresponding budget figures for 1996 and the 1994–95 biennium, to the nearest one thousand USD. There is also an estimate for 1997 based on the six-month management accounts and estimates of the costs still to be incurred by the move of the Secretariat to the Research Triangle Park, North Carolina.

	Actual	Budget
1994	149	122
1995	113	(180)
1994–95	262	(58)
1996	634/290	161
1997E	(330)	(161)
1996–97E	304/(40)	0

NB brackets denote a deficit, E denotes an estimate.

1994–95 Biennium. I have given in detail the reasons for the departures from budget for the years 1995 and 1996 in my commentary to those years' accounts in the July issues of *CI*, but let me summarize the principal factors. In 1995 the biggest contributor to the departure from budget was an underspend of USD 161k on the Guildford Assembly, mainly brought about because only 85% of TMs attended and because, contrary to what had been expected, there was broadly no inflationary increase in airfares between 1993 and 1995. Another large contributor was an underspend of USD 62k by the Divisions and Standing Committees. Had the Guildford Assembly cost the budgeted USD 490k and had the Divisions and Standing Committees spent their allocations, the result would have been a modest surplus of USD 30k for the biennium. As it was, a small increase over budget in 1994 of USD 27k led to an overall result for the 1994–95 biennium of USD 262k, markedly higher than the budgeted deficit of USD 58k.

1996–97 Biennium. During 1996, there was an expected addition to the Union's funds from Barings Brothers Bank. 'Office International de Chemie' which was

part of the Union when it was created in 1919, did not close its account with the bank when it ceased operating. This money with substantial accrued interest has been paid to the Union as successor, a sum of USD 344k.

It is now part of the reserves but accountancy rules demand that it should go through the 1996 Income and Expenses account so swelling the 1996 surplus. Even so, the surplus without it is still USD 290k, USD 129k better than budget, a result brought about largely by a Publications surplus of USD 61k over budget and an underspend of USD 30k on the Affiliate Membership Programme, both results due mainly to unexpected resignations of staff with consequent reductions in staff costs. There will be, however, consequent increases in Publications staff costs in 1997. A healthy number of smaller contributions make up the balance.

In attempting an estimate for 1997 a number of unbudgeted items, some large, have to be taken into account. These items although unbudgeted were thoroughly discussed and approved by the Executive Committee and the Bureau, recognizing that our reserves are strong and intended to be used for such eventualities. These items arise from two sources, first, the extra meetings to discuss how best to increase the relevant visibility and appeal of the Union's work to the chemical industry as well as to the rest of the chemical community, and secondly, the move of the Secretariat to the Research Triangle Park, North Carolina, USA. The extra meetings, two of which were with eminent figures from industry and academia in Europe and Asia will cost some USD 30k. Redundancy payments to the Oxford

staff will amount to about USD 130k. Recruiting and appointing the new Executive Director plus staff and other costs resulting from running two offices for five months will amount to about USD 100k. Together with an adjusted figure for the budgeted deficit, the estimated deficit is about USD 380k. But despite earlier concern about the cost of the 1997 Assembly, the eventual cost may be USD 50k below budget, giving a total deficit for the year of USD 330k. If the Barings' money is included in the 1996 surplus there will be a biennial surplus of about USD 304k. If, more realistically, this money is taken out, the result is a deficit of USD 40k. The cost of equipping the new office this year will be about USD 55k, but this being capital it can be taken straight to the Balance Sheet and thus come directly from reserves.

The substantial surplus made in the 1994–95 biennium and the good improvement over budget in 1996 is a continuing indication that we have emerged from the difficult financial position of the early nineties about which I shall have more to say later. Provided that we keep the same careful control of expenses and maintain the real value of our income by keeping subscriptions in line with inflation, it will be possible to keep a balanced budget in the years to come. It is unlikely that the circumstances that gave rise to the recent surpluses will reoccur. The next three General Assemblies are in expensive venues, Geneva, Berlin and Brisbane and the new initiatives which should result from present discussions about the Union will require the maximum of resources.

Reserves. The recent surpluses and the good returns we have been able to secure from our investments have strengthened our general reserve. In 1996, excluding the Building Fund and the Southern Hemisphere Sinking Fund, it increased in value from USD 2451k to USD 3093k.

It is proposed to use the Barings' money, USD 344k, to found a separate Endowment Fund, the interest from which to be used for special purposes. The capital needed to equip the new Secretariat offices, the 1997 deficit and removal of the Barings' money will reduce the main reserve to USD 2364k but this is still substantially above the target figure for reserves so that there is good opportunity to use the excess for one-off or short-term endeavours of the type that could emerge from the present discussions about new initiatives.

The several additions made at various times during the year—the decision to use the same investment strategy for the Building Fund as used for the general reserve, the transfer of USD 100k from the cash account to the Building Fund, the conversion of other monies in this account to stocks and shares and the addition of the Barings' money—make it very difficult to deduce a figure for the total performance of the investments during 1996. But if we take the investments which were held for the whole year, some 85% of the final sum, the equity portion gained 24% and the bond portion 4.9%, with a combined gain of 19%. Several bonds matured during the year and only four remained throughout the year. If we assumed the gain on them all was also 4.9%, the combined gain can be calculated as 17%. It should be emphasized that this figure is indicative only.

The Building Fund, which since March 1996 has the same proportion of equities to bonds as the main reserve, an average of 55:45 and to which was added USD 100k in March, gained only 9% in value. This was because the Fund had been held in British equity and bond unit trusts at the beginning of the year and these had to be sold at a loss to buy the dollar mutual funds in order to follow the investment strategy used for the main reserve.

In summary

By carefully controlling expenditure and maintaining the real value of subscriptions, the Union has corrected the imbalance between income and expenditure that led to the dire financial forecasts of 1991 and the subsequent deficits. In addition our reserves are strong and at a level that will enable substantial sums to be spent on short-term initiatives. This strength should not lead Council to neglect the duty to keep the level of subscription income in line with increases in the retail price index, as practised by almost all organizations, companies and shops. It was the failure to do so in the second half of the 1980s that was one of the principal causes of the financial difficulties that are now behind us, and that must remain there.

Treasurer's Review 1991–1997

J.M. Ward

Income and expenses

At the General Assembly in Hamburg, 1991, I presented, as Chairman of the Finance Committee, a financial forecast for the following four years. Two methods of forecasting were used, one based on projecting regression lines of the results for income and expenses for the preceding four biennia and another based on assumptions about future economic projections. There was satisfactory agreement between the two forecasts which showed that if the past trends continued there would be a cumulative deficit over the next two biennia, i.e. 1992–95, of over one million US-dollars.

The principal reasons for this imbalance between expenses and income were first a failure by Council to agree to keep subscription income at least in line with inflation, and secondly a levelling off after 1985 of contributions from the other main sources of income, investments and publications, an eventuality that the Finance Committee had warned against but which warning had gone unheeded. In 1982–83 subscriptions amounted to 80% of total income, in 1987–88 the proportion had fallen to 55% and had then remained more or less constant.

At its meeting before Council the Bureau agreed to take action and made substantial cuts in budgeted expenses, principally a cut of 12% in the allocation to Divisions, and it recommended an increase in subscriptions of 5% for each of the years 1992 and 1993. Council agreed to the increases.

When I became Treasurer on 1 January 1992 my main concern then was to restore the cuts in the Divisional allocation while maintaining a balanced budget. To do this it was necessary to keep strict control of expenses, and all parts of the Union assisted me in this, and to persuade Council to maintain the real value of our subscriptions. Again, in spite of difficulties in some countries, Council has supported my recommendations.

In 1991 the income and expenses account showed a deficit of USD 162k, which but for a change in accounting convention recommended by the auditors, would have been a deficit of USD 256k. In 1992 the deficit fell to USD 72k. In 1993 the financial measures achieved their purpose and there was a small surplus of USD 23k. In the following year, 1994, there was a further small surplus over budget of USD 27k. There was a further true surplus over budget in 1996 of USD 129k—USD 473k if the Barings windfall was included. Heavy expenses in 1997 will probably result in a biennial deficit of USD 40k.

In summary, the bottom lines of the income and expenses accounts from 1990 to 1996, in thousands of USD, are as follows (an estimate for 1997 is also given).

1990	1991	1992	1993	1994	1995	1996	1997E
12	(162)	(72)	23	149*	113	291	(330)

The biennial figures are

1990–91	1992–93	1994–95	1996–97E
(150)	(49)	262	(40)

N.B. brackets denote a deficit, E denotes an estimate.

*Under the accounting convention now used for a balanced budget, a surplus in the even year is balanced by an equal deficit in the odd (Assembly) year. This accounts for the difference between 149k and the figure of 27k for the difference between actual and budget figures given in the text.

The divisional allocation

Returning to the objective of restoring the cuts made in the Divisional allocation at the Hamburg Council Meeting, although I was able to maintain the Divisional allocation at the 1992 level over the first few years, whereas the allocation to Standing Committees was reduced, the 1994–95 allocation was 18% below the pre-Hamburg value in real terms. Council has continued to agree to subscription increases in line with inflation, and this figure fell to 15% in 1996–98. If the recommendation for a 3% increase in 1998 and 1999 is accepted, the Divisional allocation will have been restored. The details are, in thousands of USD:

	Allocation	Pre-Hamburg allocation, adjusted*
1992–93	301	342
1994–95	301	365
1996–97	331	389
1998–99	420	415

*Adjusted to take account of increases in OECD retail price indices. The OECD figures used are those for the beginning of the years 1992, 1994, 1996 and 1998, the years when the allocations were made. A forecast figure of 3.0% is used for 1997 to give the figure for the beginning of 1998.

Finally, subscription income accounted for 66.5% of total income in the 1995–96 biennium compared with

57% in 1990–91. If the 3% increase in subscriptions is agreed the budgeted income for the biennium 1998–99 will be 69% of total income. As mentioned above, in 1982–83 it was 80%.

The reserves

Although the Union has been in difficulties with its annual income and expenses account, it was not in real financial danger because the reserves were strong. These have remained so and the following summary in thousands of USD shows the value of reserves over the years 1991-1996. The values are book values. The 1996 market values are shown in square brackets.

	General reserve	Building Fund	Southern Hemisphere	Total
1991	2182			2182
1992	2156	319		2475
1993	2082	333		2415
1994	2366	289		2655
1995	2362	303		2665
1996	2520* [2749]	396 [440]	50	2966 [3239]

*Excluding the USD 344k Barings' money.

If the 1991 figure is adjusted for OECD inflation between 1991 and 1996, its value becomes USD 2568k, so it could be said that the general reserve has remained constant in book value; the market value has risen by 7%. Since 1991 the Building Fund and the Southern Hemisphere Sinking Fund have been established—if these are included the book value of the total reserves is USD 2966, an increase since 1991 of 15%; in market value the total reserves in real terms have increased in value by 26%. Since the Barings' money is a windfall not in any way earned by the Union, I have not included it in the calculations, nevertheless, it is now part of our reserves.

The target value of the general reserve, which is the sum of the last two years' expenses, was USD 2007k at the end of 1996, so that the book value of the general reserve is USD 514k above it; the market value is USD 742k above it. By the end of 1997 these sums will be reduced by the USD 55k needed for capital equipment for the new Secretariat office and by the 1997 deficit which could be as much as USD 330k. On the other hand the market value should be enhanced by capital gains in our holdings of equities and bonds. All in all, there are ample monies for important and urgent short-term initiatives and the Union should take advantage of the opportunity during the next few years.

Conclusion

The finances of the Union are now well under control, both the operational finance and the level of reserves. This latter gives opportunities to undertake special short-term initiatives and these opportunities must not be missed. I hope and trust that Union Members will give my successor the support given to me by keeping careful control of spending and will continue and intensify efforts to increase income. In particular, Council should continue to maintain the real value of national subscription income.

Relocation of IUPAC Archival Material

Dr Mo Williams

Following the transfer of the archival records of the Commission on Atomic Weights and Isotopic Abundances (II.1) to the Chemical Heritage Foundation (CHF)* during 1992, the Executive Committee of IUPAC accepted an invitation from CHF to serve as an archive for other IUPAC documentation.

As a consequence of the move of the IUPAC Secretariat from Oxford (UK) to Research Triangle Park, North Carolina (USA), which is scheduled to be completed by the end of October 1997, the archives material presently held at Oxford is being sorted into two categories:

1. Current documentation to be sent to RTP
2. All other archival material to be sent to CHF (Philadelphia, USA)

In due course, it is hoped to publish a complete listing

The former First National Bank, Philadelphia, now home of the Chemical Heritage Foundation

of the material relocated at CHF. Meanwhile, the following material was sent to Philadelphia in late 1996:

Bureau: 1940–1948

Commission on Biochemical Nomenclature: 1930–1951, 1966–1970

Publications: 1919–1931, 1968–April 1969

Committee on Teaching of Chemistry: 1968–1969

Finance Committee: 1964–1972

Physical Chemistry Division (I)

—Physical Chemistry Division Committee: March 1964–December 1973

—Commission on Physicochemical Symbols, Terminology, and Units (I.1): 1932–1967, 1970

—Commission on Thermodynamics (I.2): 1936–1950, 1960–1971

—Commission on Electrochemistry (I.3): 1930–1948, April 1962–May 1970

—Commission on Physicochemical Measurements and Standards (I.4): 1919–1941, 1946–1951, 1968–1970

—Commission on Molecular Structure and Spectroscopy (I.5): 1963–1966

—Commission On Colloid and Surface Chemistry (I.6): December 1960–October 1969

Inorganic Chemistry Division (II)

—Commission on Nomenclature of Inorganic Chemistry (II.2): 1919–1971

—Commission on High Temperatures and Refractories (II.3): 1958–1959, 1965–1971

Organic Chemistry Division (III)

—Commission on Nomenclature of Organic Chemistry (III.1): 1919–1955

—Commission on Chemical Plant Taxonomy (III.2): 1968–1973

—Commission on Photochemistry (III.3): 1969

Analytical Chemistry Division (V)

—Analytical Chemistry Division Committee: January 1959–1970

—Commission on Analytical Reactions and Reagents (V.1): 1935–1950, 1964–1966

—Commission on Microchemical Techniques and Trace Analysis (V.2): 1950–1958, 1960–1969

—Commission on Equilibrium Data (V.6): 1967–1971

—Commission on Radiochemistry: 1919–1935

Applied Chemistry Division (VI)

—Applied Chemistry Division Committee: 1919–1944

—Section on Food Chemistry (VI.1): 1919–1946

—Section on Fermentation Industries (VI.2): August 1965–1969

—Section on Oils and Fats (VI.3): 1922–1954, 1958–1970

—Section VI.4: 1919–1936

—Section on Pulp Paper and Board/Reclamation of Solid Wastes: 1959, 1968–1971

—Section on Water Sewage and Industrial Waste (VI.8): June 1969

Clinical Chemistry Section

—Commission on Automation and Clinical Chemical Techniques (VII.1): August 1969

National Adhering Organizations

—Argentina: 1920–1969

—Australia: 1920, 1922

—Belgium: 1925–1971

—Canada: February 1920–May 1969

—Chile, Columbia, Cuba: 1920–1962
—Czechoslovakia: January 1970–July 1971
—Finland, Denmark: 1926–1956
—France: September 1932–July 1969
—Germany: 1922
—Greece: 1920
—Hungary, India, Ireland: July 1930
—Israel: April 1956
—Italy: January 1920–November 1969
—Japan: April 1920–March 1971
—Mexico: 1920
—Netherlands: February 1920
—New Zealand: February 1921
—Poland: June 1919
—Representatives of Portugal, China, Korea, Vietnam: April 1920
—Republic of South Africa: December 1920
—Romania: April 1920
—Spain: April 1920
—Sweden: 1920
—Switzerland: January 1920–May 1971
—Turkey, United Arab Republic: September 1956
—UK: January 1920–May 1971
—USA: January 1920–1971
—USSR (Estonia & Latvia): July 1927–April 1940
—Venezuela, Yugoslavia: April 1920

Company Associates Scheme:
—January 1969–December 1969

Council
—XXV Council (Cortina D'Ampezzo: July 1969)

Congresses
—IX: 1920–1940
—X:1936–1938
—XI: 1946–1949
—XVI: March 1956–January 1957, July 1957, September–February 1957

Conferences
—New York, USA: 1951

ICSU
—1920–1935, 1945–1951, 1964–1965, 1965–1970
—Bulletins: 1955

General
—1919–1945
—Commission Des Constantes Radioactives: 1930–1951
—*Ad hoc* Committees—Applied Chemistry, Interdisciplinary Matters: 1969–1971
—Membership of IUPAC Units: 1969
—Machine Documentation in the Chemical Field: 1946–1959
—Coordination Committee: 1966–1969
—Miscellaneous: 1919–1925
—Account Budgets: 1920
—Accounts Banks and Cash: 1935–1943
—Executive Committee Numbers, Miscellaneous, International Circulars: 1932–1950
—IOAch: May 1968
—Joint Commission on Standards, Units and Constants of Radioactivity: 1945–1950
—UN and UNESCO: 1946–1954
—IUPAC and NAO Subscriptions: 1925
—Section on Medicinal Chemistry (III.4): 1969–1970
—Commission on Statutes and Bylaws: 1938–1973
—Correspondence: 1919–1936, 1950–1955, 1968–1969.

*For an account of the origins of CHF, its mission and operating structure, governance, etc., please see *Chem. Intl.* 1995, **17**(5) (September), 166–169. CHF is an Associated Organization of IUPAC.

For further information please contact Elizabeth Swan (Director of Library Services) at the Chemical Heritage Foundation, 315 Chestnut Street, Philadelphia, PA 19106-2702, USA. Tel.: +1 (215) 925 2222 ext. 226; E-mail: eswan@chemheritage.org

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry*.

Methods for the analysis of transient absorbance data (Technical Report)

Synopsis

Procedures for the generation and collection of transient UV-visible absorbance data are briefly reviewed. Problems associated with signal generation (scattered

light, inhomogeneous distribution of transients, instability of pulsed light sources), signal detection (averaging, filtering) and signal analysis in kinetic and spectrographic flash photolysis are addressed. Methodology for the fitting of model functions to absorbance data that depend on up to three variables (time, wavelength and, e.g. temperature) is discussed.

This report was prepared for publication by Roland Bonneau (LA 348 du CNRS, Université de Bordeaux I, F-33405 Talence Cedex, France), Jakob Wirz (Institut für Physikalische Chemie, Universität Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland) and Andreas D. Zuberbühler (Institut für Anorganizche Chemie, Universität Basel, Spitalstrasse 51, CH-4056 Basel, Switzerland) for the Commission on Photochemistry of the Organic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 979–992.*

Molecular characterization of commercial polypropylene with narrow and broad distribution of molar mass (Technical Report)

Synopsis

The molar mass and the molar mass distribution of two commercial grades of isotactic polypropylene, Moplen S30S of Himont Srl and Daplen PT55 of PCD Polymere GmbH, were investigated by 16 laboratories. For Moplen S30S M_w = 467 kg/mole ± 6.0% (relative standard deviation), M_n = 83.7 kg/mole ± 9.8% and M_w/M_n = 5.70 ± 10.1% were determined by size exclusion chromatography (31 SEC runs), for Daplen PT55 M_w = 206 kg/mole ± 13.6%, M_n = 61.4 kg/mole ± 13.4% and M_w/M_n = 3.42 ± 17.3% were found (38 SEC runs). Light scattering measurements gave M_w = 445 kg/mole ± 4.1% for Moplen S30S (4 labs) and M_w = 212 kg/mole ± 10% for Daplen PT55 (3 labs). The intrinsic viscosity in 1,2,4-trichlorobenzene at 140 °C of Moplen S30S [η] = 1.87 dl/g ± 5.4% and of Daplen PT55 [η] = 1.12 dl/g ± 6.7% was measured (nine independent measurements). Samples of the respective lots are available from the authors, Moplen S30S from IM, Daplen PT55 from KL.

This report was prepared for publication by K. Lederer (Institut für Chemie der Kunststoffe, Montanuniversität Leoben, A-8700 Leoben, Austria) and I. Mingozzi (Himont Italia, Centro Ricerche G. Natta, I-44100 Ferrara, Italy) for the Working Party on Molecular Characterization of Commercial Polymers, Commission on Polymer Characterization and Properties, Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 993–1006.*

Reference Value Standards and Primary Standards for pH measurements in D_2O and aqueous-organic solvent mixtures: New accessions and assessments (Technical Report)

Synopsis

Recommended Reference Value Standards based on the potassium hydrogen phthalate buffer at various temperatures are reported for pH measurements in various binary solvent mixtures of water with eight organic solvents: methanol, ethanol, 2-propanol, 1,2-ethanediol, 2-methoxyethanol ('methylcellosolve'), acetonitrile, 1,4-dioxane and dimethyl sulfoxide, together with Reference Value Standards based on the potassium deuterium phthalate buffer for pD measurements in D_2O. In addition are reported Primary Standards for pH based on numerous buffers in various binary solvent mixtures of water with methanol, ethanol and dimethyl sulfoxide, together with Primary Standards for pD in D_2O based on the citrate, phosphate and carbonate buffers.

This report was prepared for publication by P. R. Mussini, T Mussini and Sandra Rondinini (Department of Physical Chemistry and Electrochemistry, University of Milan, 20133 Milano, Italy) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1007–1014.*

Properties and units in the clinical laboratory sciences. II: Kinds-of-property (IUPAC Recommendations 1997)

Synopsis

The document circumscribes the concept 'kind-of-property' (property in a general sense) and lists the kinds-of-property mostly used in the clinical laboratory sciences. The concepts are as defined in the 'Compendium of terminology and nomenclature of properties in clinical laboratory sciences', except for a few that are defined intuitively. Each is given a unique code value and is expressed in different languages for use in the assembly of terms representing individual properties.

This report was prepared for publication by Desmond Kenny (Our Lady's Hospital for Sick Children, Crumlin, Dublin 12, Ireland) and Henrik Olesen (Department of Clinical Pharmacology, Copenhagen University Hospital, Copenhagen, Denmark) for the Committee on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1015–1042.*

Properties and units in the clinical laboratory sciences. V: Properties and units in thrombosis and haemostasis (Technical Report)

Synopsis

For historical reasons, the elements of properties (terms) used in the nomenclature for properties in thrombosis and haemostasis differ according to 'school' of thought. This hampers communication. In collaboration, the Scientific and Standardization Committee of the International Society on Thrombosis and Haemostasis and the Commission (Committee) of Nomenclature, Properties and Units, previously 'Quantities and Units', have prepared a set of recommended systematic names for properties in that domain. For use in electronic transmission each property has been given a code value. The prefix to the code values has been changed from 'QU' to 'NPU' because of the change of name of the Commission (Committee).

This report was prepared for publication by M. Blombäck (Department of Clinical Chemistry and Blood Coagulation, Karolinska Hospital, Stockholm, Sweden), R. Dybkaer (Department of Clinical Chemistry, Frederiksberg Hospital, Copenhagen, Denmark), K. Jørgensen (Department of Clinical Biochemistry KB 3011, Copenhagen University Hospital, Copenhagen, Denmark), H. Olesen (Department of Clinical Pharmacology Q 7642, Copenhagen University Hospital, Copenhagen, Denmark) and S. Thorsen (Department of Clinical Biochemistry KB 3011, Copenhagen University Hospital, Copenhagen, Denmark) for the Commission on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division (in collaboration with the Scientific and Standardization Committee of the International Society on Thrombosis and Haemostasis). The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1043–1079.*

Properties and units in the clinical laboratory sciences. VI: Properties and units in IOC prohibited drugs (Technical Report)

Synopsis

The term designating a substance being an active ingredient of a drug may be a generic name, a non-proprietary name, a registered trade name, a fantasy name or other. This causes difficulties in the transmission of request and report on such substances to and from the clinical laboratories, and in the collating of this information from different sources. The document comprises a list of properties of drugs of abuse in biological fluids as defined by the International Olympic Committee Medical Code for use in electronic transmission systems. Standard systematic names are presented with a code value for each. The coding schemes thus prepared are accessible on the Internet from the Commission on Nomenclature, Properties and Units' Home Page address: http://inet.uni-c.dk/~qukb7642.

This report was prepared for publication by H. Olesen (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark), D. Cowan (Drug Control Centre, London University, King's College, London, UK), I. Bruunshuus (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark), K. Klempel (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark) and G. Hill (Department of Clinical Chemistry, Hospital for Sick Children, Toronto, Ontario, Canada) for the Commission on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1081–1136.*

Glossary of terms used in computational drug design (IUPAC Recommendations 1997)

Synopsis

Computational drug design is a rapidly growing field which is now a very important component in the discipline of medicinal chemistry. At the same time many medicinal chemists lack significant formal training in this field and may not have a clear understanding of some of the terminology used but need to grasp concepts, follow research results, define problems for, and utilize findings of, computational drug design. In this context the IUPAC Medicinal Chemistry Section Committee felt it would be useful to develop a glossary of terms used in computational drug design for easy reference purposes. Also there is the possibility that in different countries certain terms may not have the same meaning and in such a case there would be value in trying to establish an international definition standard. Accordingly a Working Party of seven experts in the field was assembled who constructed a glossary of some 100 terms. Concise but sufficiently explanatory definitions have been formulated based on a variety of literature sources and selected key references provided.

This report was prepared for publication by H. van de Waterbeemd, Chairman (F. Hoffmann-La Roche, Pharma Research New Technologies, CH-4070 Basel, Switzerland), R.E. Carter (Astra Hässle AB, Computational Chemistry, S-43183 Mölndal, Sweden), G. Grassy (Centre de Biochimie Structurale, Faculté de

Pharmacie, F-34060 Montpellier, France), H. Kubinyi (BASF AG, ZHB/W A30, D-67056 Ludwigshafen, Germany), Y.C. Martin (Abbott Laboratories, Computer-Assisted Molecular Design, Abbott Park, IL 60064-3500, USA), M.S. Tute (University of Canterbury, Kent CT2 7NH, UK) and P. Willett (University of Sheffield, Department of Information Studies, Sheffield S10 2TN, UK) for the Medicinal Chemistry Section of the Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1137–1152.*

Intrinsic characterization of continuous carbon fibre thermoplastic composites. 3: Fatigue crack growth (Technical Report)

Synopsis

This paper reports some fatigue crack growth results obtained on unidirectional laminates of AS4/PEEK. Crack growth is intralaminar and the study has included the influence of laminate thickness, method of consolidation and level of applied stress level. Presentation of data is by a Paris Law type approach, where crack growth per cycle is plotted against a stress field intensity factor. The measurements have involved four different laboratories and therefore it has been possible to attempt to embrace the likely scatter involved in the collection of fatigue data commensurate when several laboratories conduct seemingly similar measurements.

This report was prepared for publication by D.R. Moore (ICI plc, Wilton, Middlesbrough, Cleveland, UK) and J.C. Seferis (Polymeric Composites Laboratory, University of Washington, Seattle, USA) for the IUPAC Working Party IV.2.1: Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1153–1161.*

Guidelines for publication of equations of state. I: Pure fluids (Technical Report)

Synopsis

During recent decades equations of state have become a major tool for the correlation and prediction of thermodynamic properties of fluids. Equations of state can be applied to pure substances as well as to mixtures, and therefore a very large number of publications deal with the development or improvement of equations of state. In order to give authors, editors and reviewers of publications on new equations of state some guidelines and to ensure that future publications will be more profitable for the reader, some criteria for pure fluids are given that ought to be fulfilled by a good manuscript.

This report was prepared for publication by U.K. Deiters (Institut für Physikalische Chemie, Universität zu Köln, D-50939 Köln, Germany) and K.M. de Reuck (Chemical Engineering Department, Imperial College of Science, Technology & Medicine, London SW7 2BY, UK) for the Commission on Thermodynamics of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1237–1249.*

Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997)

Synopsis

The glossary contains definitions and (where needed) explanatory notes for about 400 terms used in the multidisciplinary field of bioinorganic chemistry. A need has been recognized for globally acceptable definitions of terms in this field and this glossary was compiled with the objective of fulfilling this need. It is by no means a comprehensive dictionary. The terms selected were those considered essential and/or widely used. The definitions given reflect current usage and complement IUPAC guidelines. Abbreviations and acronyms, frequently used in bioinorganic chemistry, are included.

This report was prepared for publication by M.W.G. de Bolster (Vakgroep Organische en Anorganische Chemie, Faculteit der Scheikunde, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands) for the Working Party on IUPAC Glossary of Terms Used in Bioinorganic Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1251–1303.*

Characterization of SiC powders and the influence of powder properties on sintering (Technical Report)

Synopsis

This report summarizes the characteristics of SiC powders which influence the ability to obtain fully dense (non-porous) ceramics, with good mechanical properties, via the sintering process. Methods for characterizing powder properties, such as particle size, morphology, bulk and surface chemistry, are outlined and specific examples are referenced. The characteristics of typical commercial SiC powders are tabulated.

This report was prepared for publication by G. Schwier and I. Teusel (H.C. Starck GmbH & Co. KG, D-38642 Goslar, Germany) and M.H. Lewis (Centre for Advanced Materials, University of Warwick, Coventry CV4

7AL, UK) for the Commission on High Temperature Materials and Solid State Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1305–1316.*

Chemically modified electrodes: Recommended terminology and definitions (IUPAC Recommendations 1997)

Synopsis

Chemically modified electrodes (CMEs) comprise a relatively modern approach to electrode systems that finds utility in (1) a wide spectrum of basic electrochemical investigations, including the relationship of heterogeneous electron transfer and chemical reactivity to electrode surface chemistry, electrostatic phenomena at electrode surfaces and electron and ionic transport phenomena in polymers, and (2) the design of electrochemical devices and systems for applications in chemical sensing, energy conversion and storage, molecular electronics, electrochromic displays, corrosion protection and electro-organic syntheses. Compared with other electrode concepts in electrochemistry, the distinguishing feature of a CME is that a generally thin film of a selected chemical is bonded or coated onto the electrode surface to endow the electrode with the chemical, electrochemical, optical, electrical, transport and other desirable properties of the film in a rational, chemically designed manner. In this report, the authors have attempted to identify and define the most widely used terminology in the growing field of CMEs and to recommend a particular term in cases where a multiplicity of terms has arisen over the past several years or where previously defined terms have taken on broadened meanings for the special cases of CMEs.

This report was prepared for publication by R.A. Durst (Analytical Chemistry Laboratories, Cornell University, Geneva, NY 14456, USA), A.J. Bäumner (Institute for Technical Biochemistry, University of Stuttgart, D-70569 Stuttgart, Germany), R.W. Murray and R.P. Buck (Department of Chemistry, University of North Carolina, Chapel Hill, NC 27514, USA) and C.P. Andrieux (Laboratoire d'Électrochimie Moléculaire, Université de Paris 7, 75251 Paris Cedex 05, France) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1317–1323.*

Consistency of pH standard values with the corresponding thermodynamic acid dissociation constants (Technical Report)

Synopsis

With the simplest possible assumptions on the ion activity coefficients, namely a Debye–Hückel approach, pH values of eleven standard buffer solutions have been calculated from the corresponding thermodynamic acidity constants, $K_{(I\to 0)}$, and compared to the electrometrically assigned pH(S) values (by Harned cell method). Agreement is within ± 0.01 in the temperature range 10–40 °C for all standards, except carbonate. The results for the phthalate, acetate, phosphate and carbonate systems at 25 °C indicate that this consistency is improved if specific ion interactions are taken into account, according to the Pitzer theory.

This report was prepared for publication by M. Filomena Camoes and M.J. Guiomar Lito (Centro de Electroquímica e Cinética da Universidade de Lisboa, 1294 Lisboa Codex, Portugal), M. Isabel A. Ferra (Universidade da Beira Interior, 6200 Covilhã, Portugal) and Arthur K. Covington (Department of Chemistry, University of Newcastle, Newcastle-upon-Tyne, NE1 7RU, UK) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1325–1333.*

Chirality in synthetic agrochemicals: Bioactivity and safety consideration (Technical Report)

Synopsis

Most synthetic agrochemicals with chiral structures are marketed as racemates even though the desired biological activity may be derived from only one enantiopure isomer. However, some synthetic agrochemicals such as pyrethroid insecticides, aryloxypropanoate herbicides and triazole fungicides are marketed as the most biologically active enantiopure isomer. Numerous reports describing the relative biological activities, preparations and analyses of enantiopure agrochemicals are available. Some examples of how different enantiomers in racemates are selectively metabolized have also been reported. When agrochemicals have chiral structures, efforts should be made to define the mode of action, elucidate metabolic pathways and to define the human and environmental toxicity of each enantiopure isomer. If there are large differences in the biological activities of individual enantiomers in racemates, it is desirable to develop and use only the enantiopure isomer with the highest

sought-after biological activities.

This report was prepared for publication by N. Kurihara (Radioisotope Research Center, Kyoto University, Kyoto 606-01, Japan), J. Miyamoto (Sumitomo Chemical Co. Ltd, Osaka 541, Japan), G.D. Paulson (US Department of Agriculture, ARS, Fargo, ND 58105, USA), B. Zeeh (BASF AG, Agricultural Research Station, D-67114 Limburgerhof, Germany), M.W. Skidmore (Zeneca Agrochemicals, Jealotts Hill, Bracknell, Berks., RG42 6EY, UK), R.M. Hollingworth (Pesticide Research Center, Michigan State University, East Lansing, MI 48824, USA) and H.A. Kuiper (State University for Quality Control of Agricultural Products, Rikult-Dlo Wageningen, The Netherlands) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1335–1348.*

Pesticide fate in tropical soils (Technical Report)

Synopsis

Pesticide use is an important component of agricultural and non-agricultural pest control in tropical areas. However, the fate of pesticides in tropical soils is not as well understood as that for soils from temperate regions. Tropical soils defy easy generalizations, but they are typically very old soils characterized by year-round uniformity of temperature regime. Although only a few studies have directly compared pesticide fate in tropical and temperate soils, there is no evidence that pesticides degrade more slowly under tropical conditions. Laboratory studies in which soils have been held under standardized conditions reveal that pesticide degradation rate and pathway are comparable between tropical and temperate soils. However, field investigations of tropical pesticide soil fate indicate that dissipation occurs more rapidly, in some cases much more rapidly, than for pesticides used under similar temperate conditions. The most prominent mechanisms for this acceleration in pesticide dissipation appear to be related to the effect of tropical climates, and would include increased volatility and enhanced chemical and microbial degradation rates on an annualized basis.

This report was prepared for publication by K.D. Racke (DowElanco, Indianapolis, IN, USA), M.W. Skidmore (Zeneca Agrochemicals, Bracknell, Berkshire, UK), D.J. Hamilton (Resources Sciences Centre, Indooroopilly, Queensland 4068, Australia), J.B. Unsworth (Rhône-Poulenc, Ongar, Essex, UK), J. Miyamoto (Sumitomo Chemical Company, Osaka 541, Japan) and S.Z. Cohen (Environmental and Turf Services, Wheaton, MD, USA) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1349–1371.*

Optimum use of available residue data in the estimation of dietary intake of pesticides (Technical Report)

Synopsis

Prediction of pesticide residue intake in human diets is vital for approving the use of pesticides and for gaining official acceptance of pesticide residue levels which occur in food commodities in international trade. Estimates for pesticide residue levels likely to be present in food as consumed are derived from supervised pesticide residue trials, residue monitoring, pesticide metabolism and food processing studies. The results of properly conducted total diet studies should generally displace other estimates, but they do not cover all pesticides and, in particular, are not available for a pesticide at its initial registration. Information was compiled on the range of residues occurring in a set of supervised residue trials with identical application rate, number of applications and pre-harvest interval, but at different sites with various crop varieties, operators, equipment and cultural practices. Eighteen recommendations are provided for estimating the level of pesticide residues likely to be present in food as consumed.

This report was prepared for publication by D.J. Hamilton (Resources Sciences Centre, Indooroopilly, Queensland 4068, Australia), P.T. Holland (Horticulture and Food Research Institute of New Zealand Ltd, Hamilton, New Zealand), B. Ohlin (National Food Administration, Uppsala, Sweden), W.J. Murray (Pest Management Regulatory Agency, Health Canada, Ottawa, Canada), A. Ambrus (Plant Health and Soil Conservation Centre, Budapest, Hungary), G.C. de Baptista (Departmento de Entomologia, Universidade de São Paulo, Brazil) and J. Kovacicová (Institute of Preventive and Clinical Medicine, Bratislava, Slovakia) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1373–1410.*

PAC Review

***Pure and Applied Chemistry* (PAC) is the official journal of IUPAC. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in PAC are published in *Chemistry International* in the section Recent Reports. In this section we take a brief look at symposia and lectures published in recent issues of PAC.**

Lectures from Symposia

The April 1997 issue of *Pure and Applied Chemistry* (Vol. 69, no. 4) contains the texts of lectures from three symposia: the International Symposium of Sweeteners, held in Jerusalem, Israel, on 14–20 July 1996; the 16th IUPAC Symposium on Photochemistry, held in Helsinki, Finland, on 21–26 July 1996; and the International Conference on Chemical Physics on the Border of the 21st Century, held in Moscow, Russia, on 16–19 April 1996.

Sweeteners

The International Symposium on Sweeteners was held under the auspices of IUPAC, the Hebrew University of Jerusalem and the Israel Academy of Sciences. The programme included plenary and contributory lectures from many areas of natural and synthetic sweeteners, structure–activity relationships of sweeteners, mechanism of gustation, health aspects of sweeteners, side effects of commercial sweeteners, use of sweeteners in foods, sensory characteristics of sweeteners, neurophysiological, inborn and acquired aspects of sweetness, sweeteners in weight control and diabetes and legislation of commercial sweeteners.

Prof. HRH Princess Chulabhorn Mahidol was the guest of honour at the Symposium and, at a ceremony prior to the lectures, she was presented with an Honorary Fellowship by the Hebrew University of Jerusalem. Her presentation, entitled 'Natural products for the improvement of the quality of life', covered work on the utility of some Thai plants as a source of food, including toxicological studies of stevioside and chemical investigations of cassava (*Manihot esculenta* Crantz). Her full text, plus that of the nine other plenary lectures to the conference, is presented in *Pure & Applied Chemistry*, **69**(4), 655–727.

Photochemistry

The plenary and invited lectures to the 16th IUPAC Symposium on Photochemistry [**69**(4), 729–856] as in previous years, covered a wide range of topics, including theoretical chemistry, biological chemistry, chemistry in the solid state, energy transfer and fast reaction kinetics. In particular, many examples were presented of the reactions of short-lived intermediates, such as biradicals, which exemplified their synthetic utility.

The conference concluded with the presentation of the Porter Award to Prof. Noboru Mataga of the Institute of Laser Technology, Osaka, Japan. His lecture presented results from picosecond and femtosecond laser spectroscopy studies on photoinduced transfer phenomena in solutions. Such studies have aided the development of exciplex chemistry. Topics covered included the excited dipolar solute–solvent interactions, solvent and driving force effects on the electronic and geometrical structures of inter- and intra-molecular exciplex systems, energy gap dependencies of charge separation in the fluorescence quenching reactions and charge recombination of product loose ion pairs, non-Marcus type energy gap dependence of charge recombination of compact ion pairs formed by excitation of ground state charge transfer complexes, photoinduced electron transfer coupled with proton transfer or proton shift in benzophenone-amine and some hydrogen bonding exciplex systems, and extensions of exciplex studies to photosynthetic reaction centre models.

Chemical physics

The International Conference on Chemical Physics on the Border of the 21st Century was held under the auspices of the Physical Chemistry Division in conjunction with the Russian Academy of Sciences, Moscow State University. The four plenary lectures are presented [**69**(4), 857–904], including that of the Conference Editor, Alexander E. Shilov of the Emanuel Institute of Biochemical Physics, Russian Academy of Sciences. Prof. Shilov discussed the contribution of N. N. Semenov, the 1956 joint winner of the Nobel Prize for Chemistry, to 20th century chemistry, not only of his discovery of branching chain reactions and the development of the general theory of chain reactions and thermal explosions, but also of his prediction that biology is likely to play a crucial role in future chemistry.

The other three plenary lectures dealt with: the role of

chemical physics in the science of catalysis and design of new catalytic technologies; non-traditional pathways of solid-phase astrochemical reactions; and the thermodynamics of extreme states of matter. The paper on chemical physics and catalysis was the last scientific communication by Prof. K.I. Zamaraev (immediate Past-President of IUPAC) before his untimely death in June 1996.

Solubility phenomena

The May 1997, **69**(5), issue of *Pure and Applied Chemistry* contains the texts of the plenary and specially invited lectures presented at the 7th International Symposium on Solubility Phenomena, held in Leoben, Austria, on 22–25 July 1996. The symposium was held under the auspices of the IUPAC Commission on Solubility Data, in conjunction with the University of Leoben. Nine lectures are published: Experimental studies in high temperature aqueous chemistry at Oak Ridge National Laboratory; Phase changes and chemical reactions in solid aqueous solutions; Mechanisms of crystallization and transformation of calcium carbonates; Improvement of polymer solubility—influence of shear and of pressure; Solubilities of the common L-α-amino acids as a function of temperature and solution pH; Solubility data in physicochemical data collections and databanks; Use of semi-empirical electrolyte theories for modelling of solution chemical data; Solubility data requirements and new experimental methods in atmospheric aerosol research; and Thermodynamic databases and equilibrium calculations in metallurgical processes.

Excitonic processes

The June 1997, **69**(6), issue of *Pure and Applied Chemistry* contains the texts of nine of the invited lectures presented at EXCON '96, the 2nd International Conference on Excitonic Processes in Condensed Matter, held in Kurort Gohrisch, Saxonia, Germany, on 14–17 August 1996. As Conference Editor, Michael Schreiber of the Institut für Physik, Technische Universität Chemnitz, points out, 65 years after the first papers on excitons by Frenkel, research on excitons has now developed into a truly multidisciplinary field. Excitons play a key role in excitation and energy transfer processes in many molecules, molecular aggregates and crystals, as well as in macromolecular and biological systems.

Included is a selective personal perspective on exciton research, presented by R.S. Knox of the Department of Physics and Astronomy and Rochester Theory Center for Optical Science and Engineering, University of Rochester, New York state. Exciton studies have progressed through many stages that correspond to those in atomic studies, including electronic structure, interactions with other particles, determination of oscillator strengths and ionization rates, bonding into excitonic molecules, condensation and thermal equilibration. Driven by huge advances in computation and experimental techniques, exciton research has essentially evolved from a study of structures to a study of dynamics, Prof. Knox told delegates. 'After 65 years, the exciton survives as neither a museum piece for textbooks nor a purely spectrographic detail. It continues to challenge both theorists and experimentalists, it has attained considerable technological significance, and it participates decisively at the very beginning of earth's food chain', he concludes.

The other published lectures include: Dynamics and instabilities of an exciton in the phonon field and the correlated absorption–emission spectra; Excitons in semiconductor nanostructures with disorder; Spin splittings in nanostructures without inversion symmetry; Hawking process in solids—quantum generation of phonon bursts by a strongly excited mode; Non-linear phenomena in organic multilayers; Photosynthetic light-harvesting; Relaxation processes and self-trapping of excitons in rare gas solids; and Parity-broken and -unbroken self-trapped excitons in alkali halides.

News

Measurement technologies in atmospheric chemistry

A workshop and short course on 'Instrumentation and Measurement Methodologies in Atmospheric Chemistry' was conducted during the two weeks 4–15 November 1996 at the Laboratory of Environmental Analytical Chemistry of the Federal University of Bahia, in Salvador (Bahia), Brazil. The course was organized and coordinated by Prof. Tania Tavares, Head of the Laboratory and a Titular Member of the IUPAC Commission VI.2, Atmospheric Chemistry. Several other members of the Commission also took part by serving as lecturers and/or demonstrators.

The objective of the workshop was to broaden theo-

Prof. Tania Tavares in Brazil

retical and practical knowledge in atmospheric measurement techniques among professionals of different scientific backgrounds in Third World countries, especially those that are to some extent connected with WMO Global Atmospheric Watch (GAW) stations. The syllabus included morning lectures and afternoon laboratory practice, as well as a field measurement campaign at the site of the Brazilian GAW station. Subjects taught included the behaviour and reactions of atmospheric constituents, gas phase, particulate and liquid phase sampling and measurement techniques, spectroscopy, chromatography, fundamentals of quality assurance and control, and meteorological concepts required for data interpretation.

This was the first course of its kind, which offered laboratory instruction in addition to lectures. The course was open to anyone who had a good command of English and who was engaged in work related to chemical analysis of components in the air. Twenty-six persons from eight different countries attended: Argentina, Brazil (four different states), Chile, Costa Rica, Indonesia, Kenya, Mexico, Puerto Rico. The lecturers, who were either analytical or atmospheric chemists, aside from two meteorologists, came from Brazil, Croatia, Germany, The Netherlands and the USA.

Sponsors of the workshop, in addition to IUPAC's Chemistry of the Environment Division, included the American Geophysical Union (AGU), the Atmospheric Chemistry and Environment Education Committee of the International Global Atmospheric Chemistry Programme (IGAG), the Inter American Institute for Global Change Research (IAI) and the Global Change System for Analysis, Research and Training (START).

Judging from the comments of the participants, the workshop has been highly successful and fully met all the objectives. Prof. Tavares is to be thanked for a very substantial effort that made this project a success.

Peter Warneck
Chairman, Commission VI.2, Atmospheric Chemistry

CHEMRAWN in Montevideo

Prof. Patrick Moyna of the University of Montevideo writes:

As a result of extensive discussion in the CHEMRAWN Committee and with all the Chemical Societies in Latin America, there is considerable support for a CHEMRAWN-style conference to be held in Montevideo. The conference, proposed for 15–20 March 1998 under the title 'Chemical Studies Applied to Environmental Evaluations', will be aimed at improving the evaluation and understanding of changes to the environment and the implementation of sensible measures to conserve it. Montevideo is at the heart of the recently established Mercosur economic region (which includes Argentina, Brazil, Paraguay and Uruguay, and will shortly be extended to include Bolivia; there is an initial association with Chile and negotiations have begun with Peru, Ecuador, Columbia and Venezuela).

The conference goals are to enable experts in Latin America to analyse the present situation and to exchange experiences and help foster use of best practices and to prepare recommendations for future work, establish monitoring networks and build up the concepts and practice of quality assurance and control. Emphasis will be placed on the need for collaboration between government, environmental agencies, industry and academic institutions.

Support from and collaboration with other relevant IUPAC Divisions and also UNESCO, IOCD and RAQAL are considered essential for the success of the conference.

For further information, please contact: Prof. Patrick Moyna, Facultad de Quimica, University of Montevideo, CP 11800 Montevideo, Uruguay. Tel.: +598 2 94 1884. Fax: +598 2 94 1906.

COSPAR scientific assembly

The 32nd COSPAR (Committee on Space Research established by the International Council of Scientific Unions) Scientific Assembly is scheduled to be held on 12–19 July 1998 in Nagoya, Japan. The programme is intended to cover around 80 meetings and symposia, on topics including:

- The Earth's surface, meteorology and climate
- The Earth–Moon system, planets and small bodies of the Solar System
- The upper atmospheres of the Earth and planets, including reference atmospheres
- Space plasmas in the Solar System, including planetary magnetospheres
- Research in Astrophysics

- Life sciences as related to space
- Materials sciences in space
- Fundamental physics in space
- Satellite dynamics
- Scientific ballooning
- Space born geophysical data for global change studies
- Science and engineering aspects for Solar System exploration

Abstracts are invited by 9 January 1998, and papers will be published in *Advances in Space Research*.

For more information, please contact: COSPAR Secretariat, 51 bd de Montmorency, 75016 Paris, France. Tel.: +33 1 45 25 06 79. Fax: +33 1 40 50 98 27. E-mail: COSPAR@paris7.jussieu.fr. Information is also available on the WWW at http://www.mpae.gwdg.de/COSPAR/COSPAR.html.

IFCC/Roche establish Human Genomics Conferences

The International Federation of Clinical Chemistry (IFCC), an Associated Organization of IUPAC, and Roche Diagnostics have agreed to establish a series of conferences 'Human Genomics: the Basis of the Medicine of Tomorrow'. They aim to highlight progress in molecular genetics and its potential in diagnosis and therapy. The first conference, entitled 'Recent Progress in Molecular Biology Technology', is to be held in Singapore on 15–18 March 1998. This will focus on improved DNA diagnostics and define the role of the clinical chemistry laboratory of the future. The organizers wish to bring together scientists specialized in the field of molecular diagnostics for discussion and preparation of recommendations for better clinical use of these new technologies. They also plan to offer interested clinical chemists a high level course in molecular diagnostics after the Conference.

For further information, please contact: Ursula Steeb, IFCC-Roche Conference Secretary, Roche Diagnostics, Bau 223/315, Postfach, CH-4070 Basel, Switzerland. Tel.: +41 61 6872516. Fax: +41 61 687 25 10. E-mail: Ursula.Steeb@Roche.com

'Dictionary of Substances' goes online

The *Dictionary of Substances and their Effects*, produced by the UK's Royal Society of Chemistry (RSC), is now available as an online file (file 307) on Dialog, an online service of Knight-Ridder Information Inc. The online file provides a pay-as-you-go access option, complementing the print and CD-ROM versions already available from the RSC. The dictionary is a specialist reference source of toxicological and environmental data on over 4000 chemicals, updated twice a year.

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *The IUPAC Handbook 1996–1997*. The IUPAC Secretariat has been notified of the following changes:

Dr David L. Berner (Secretary, Commission on Oils, Fats, and Derivatives), 10 East Pointe, Fairport, New York 14450, USA. Tel. and Fax: +1 (716) 223 9388.
E-mail: amberner@ix.netcom.com

Dr Patrick T. Holland (Secretary, Commission on Agrochemicals and the Environment), HortResearch, Private Bag 3123, Hamilton, New Zealand. Tel.: +64 (7) 838 5045. E-mail: hollandp@hort.cri.nz

Prof. Waldfried Plieth (Chairman, Commission on Electrochemistry), Inst. für Physikalische Chemie und Elektrochemie, Technische Universität Dresden, Mommsenstraße 13, D-01062 Dresden, FRG.

Prof. Rolf D. Schmid (Chairman, Commission on Biotechnology),
E-mail: itbrsc@po.uni-stuttgart.de

IUPAC colleagues deceased

UK: Prof. G. Gee (13 December 1996), Commission on Macromolecules (1953–1961, 1965–1969).

UK: Prof. M.L. McGlashan (18 July 1997), Interdivisional Committee on Nomeclature and Symbols (1969–1975), Physical Chemistry Division Committee (1969–1973), Commission on Physicochemical Symbols, Terminology and Units (1963–1979), Commission on Thermodynamics (1965–1969).

USA: Prof. C.G. Overberger (17 March 1997), Executive Committee/Bureau (1977–1985), CHEMRAWN Committee (1976–1986), President of Macromolecular Division (1977–1979), Macromolecular Division Committee (1967–1977), Commission on Polymer Characterization and Properties (1977–1980), Commission on Macromolecules (1965–1967).

New Publication

Molecular Electronics—a 'Chemistry for the 21st Century' monograph

The study of molecular electronics has an ambitious but realistic goal, the use of synthesis, assembly and miniaturization on the molecular level to achieve a huge diversity of devices: molecular wires, rectifiers, switches, transistors and memories. It foresees applications not only in standard electronics but also some unique to molecular systems, for instance sensors based on molecular recognition, and molecular interfaces with biological systems.

Molecular Electronics recognizes its subject as a multidisciplinary area of research, tracing its origins in both physics (with attempts to replicate on the molecular level devices from solid-state electronics) and biology (where nature has arrived at organic solutions for functions such as memory and photosensitivity). The book, co-edited by IUPAC Vice-President and President-Elect Prof. Joshua Jortner, provides an up-to-date set of authoritative overviews spanning molecular electronics and assessing its future directions.

The first chapter, written by the two co-editors, serves as an introduction, providing a review of some of the goals, concepts, problems, ideas, experiments and theoretical arsenal of molecular electronics. Included is a description of the different categories of devices that have been envisioned—molecular wires, switches, memory elements, electrodes, energy conversion, sensors, optics and optical switches, displays, electrochemical devices, heterostructure and quantum-well devices, information processing, diodes and rectifiers and intrinsically novel molecular devices. The authors relate them to standard solid state systems, and point out their possible uses in actual devices. Then follows a section devoted to the basic chemical physics

Prof. Joshua Jortner

underlying much of molecular electronics, including electron transfer, proton transfer, photo absorption, non-linear optics, descriptions of localization and relaxation, and the coupling of subcomponents. An example analysis based on molecular wires is also presented. The chapter concludes with a consideration of some of the intrinsic limitations and promise of the field of molecular electronics.

Fourteen further chapters, featuring contributors from around the world, deal with topics ranging from molecular control of electron and hole transfer processes to protein-based memories and processors.

Molecular Electronics—a 'Chemistry for the 21st Century' monograph. Edited by J. Jortner, School of Chemistry, Tel Aviv University, Ramat Aviv, Israel, and M. Ratner, Department of Chemistry, Northwestern University, Evanston, Illinois, USA. Published by Blackwell Science, Osney Mead, Oxford OX2 0EL, UK, 1997. 485 pp. + viii. ISBN 0 632 04284 2. Price: USD 125; GBP 75.

Conferences

1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences, GSF-Forschungszentrum, Neuherberg/München, Germany, 4–7 May 1998

IUPAC
SPONSORED

The conference, organized by the GSF National Research Center for Environment and Health, aims to focus on the broad, new and sometimes diffuse activities relating to speciation and to create a forum for open discussions about very new and perhaps not fully established findings.

The main topics will be:

- Separation and hyphenated techniques
- Quality assurance and reference materials in

speciation analysis
- Speciation in the biomedical field
- Speciation in the environmental field
- Speciation in the nutritional field
- Speciation in occupational health
- Speciation and legislation

The conference programme will comprise three days of oral presentations, posters and extended time for discussion. Oral presentations (invited or submitted) will be 60 or 20 minutes in duration including discussion. Special poster discussions will be organized, where authors will have the possibility of presenting orally the highlights of their poster. Round table discussions will be organized on special topics (for which suggestions are welcomed). On the fourth day, four short courses will be offered: Separation methods using chromatographic techniques; Separation methods using CE techniques; Quality control in speciation analysis; and Sample preparation in speciation for different matrices and elements.

Abstracts of papers must be submitted in English (three copies) to the Chairman of the Organizing Committee by 31 October 1997.

The registration fee is DM 400 before 1 March 1998, DM 500 after 1 March 1998, for participants, and DM 200 for students. A one-day ticket is also available at DM 150. The conference dinner on 5 May is DM 100. The proceedings are DM 75. Each short course is DM 150. A combined ticket for the Speciation Conference and the 5th Conference on Metal Ions in Medicine and Biology (organized from 8 to 10 May at the GSF National Research Center in conjunction with the Hahn-Meitner Institute Berlin) is DM 800 before 1 March 1998, and DM 1000 after 1 March 1998. Members of IUPAC are entitled to a 10% reduction on the registration fee.

For further information on submission of a paper, please contact: First Speciation Conference, c/o Prof. Dr P. Schramel, GSF-Forschungszentrum, Inst. for Ecological Chemistry, Postfach 1129, D-85758 Oberschleissheim, Germany. Tel.: +49 89 31874062.

For further information on registration, please contact: First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, Germany. Tel.: +49 89 31873030/2669; Fax: +49 89 31873362.

Degradation Processes in the Environment, Dubrovnik (Cavtat), Croatia, 24–28 May 1998

IUPAC SPONSORED

The aim of the conference is to discuss the state-of-the-art in our understanding of environmental degradation processes along the following topics:
- Atmospheric degradation processes
- Degradation processes in water and soil
- Degradation data: sources and quality
- Modelling degradation processes
- Application of research results in environmental management

In particular, attention will be paid to the kinetics and reaction mechanisms, assessment of availability and quality of degradation data, and qualitative and quantitative modelling of degradation processes. It is hoped that the conference will reach recommendations on data quality standards, estimation of degradation rates, and identify the major gaps in knowledge where future research is needed.

The registration fee is USD 200 before 1 February 1998 and USD 300 after 1 February 1998. The fee will include a book of abstracts, a get-together party, morning and afternoon tea or coffee and an excursion to the historic sites of Dubrovnik. Students will have a 50% discount on the fee.

For further information, please contact: Dr Aleksandar Sabljic, Ruder Boskovic Institute, PO Box 1016, HR-10001 Zagreb, Croatia. Tel.: +385 14561089. Fax: +385 1425497. E-mail: dpe@indigo.irb.hr.

Conference Calendar

1997

Electron transfer processes

3–7 September
International Symposium on Electron Transfer Processes and Reactive Intermediates in Macromolecular and Organic Chemistry. Zabre, Poland.
Prof. Z.J. Jedlinski, Institute of Polymer Chemistry, Polish Academy of Sciences, ul. Marii Curie Sklodowskiej 34, 41-800 Zabrze, Poland. Tel.: +48 (32) 1716077; Fax: +48 (32) 1712969; E-mail: polymer@usctoux1.cto.us.edu.pl

Colloquium spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997. Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122,

Australia. Tel.: +61 (3) 98193700; Fax: +61 (3) 98195978.

Emulsions

23–26 September
2nd World Congress on Emulsions: Industrial Applications of Emulsions. Bordeaux, France.
Mr A. Le Coroller, Directeur-Général, CME, 50 place Marcel Pagnol, 92100 Boulogne-Billancourt, France. Tel.: +33 (1) 47617689; Fax: +33 (1) 47617465 .

Green chemistry

28–30 September
International Conference on Green Chemistry: Challenging Perspectives. Venice, Italy.
Conference Secretariat, Green Chemistry: Challenging Perspectives, Consorzio Interuniversitario Nazionale 'La Chimica per l'Ambiente', Facolta di Scienze Matematische, Fisiche e Naturali, Calle Larga S Marta 21.37, 30123 Venezia, Italy.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all *bona fide* chemists from throughout the world to attend irrespective of race, religion, or political philosophy. IUPAC sponsorship implies that entry visas will be granted to all *bona fide* chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

Macromolecule–metal complexes

6–10 October
7th International Symposium on Macromolecule-Metal Complexes (MMC-7). Noorwijkerhout, Netherlands.
Prof. J. Reedijk, Leiden Institute of Chemistry, PO Box 9502, 2300 RA Leiden, Netherlands. Tel.: +31 (71) 5274459. Fax: +31 (71) 5274451; E-mail: reedijk@rulgca.leidenuniv.nl

Biodiversity and bioresources

23–27 November
International Conference on Biodiversity and Bioresources—Conservation and Utilization. Phuket, Thailand.
IUPAC Biodiversity Conference, National Center for Genetic Engineering and Biotechnology, National Science and Technology Development Agency Building, 73/1 Rama VI Road, Bangkok 10400, Thailand. Tel.: +66 (2) 6448150-4, ext. 505, 532, 534; Fax: +66 (2) 6448107-8; E-mail: iupacconf@biotec.or.th

1998

Polymer sciences and technology

5–10 January
International Symposium on Advances of Polymer Sciences and Technology. Madras, India.
Dr K.S.V. Srinivasan, Deputy Director & Head, Polymer Division, Central Leather Institute, Council of Scientific & Industrial Research, Adyer, Madras - 600 020, India.

Calorimetry and chemical thermodynamics

5–9 April
International Conference on Calorimetry and Chemical Thermodynamics. Campinas, Brazil.
Prof. C. Airoldi, Instituto de Química, UNICAMP - CP 6154, Universidade Estradul de Campinas, 13081-970 Campinas sp, Brazil.
http://www.iqm.unicamp.br/wloh/conf/

Trace element speciation

4–7 May
1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences. Neuherberg, Munich, Germany.
First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, FRG. Tel.: +49 (89) 31873030 (2669); Fax: +49 (89) 31873362.

Degradation processes in the environment

24–28 May
International Conference on Degradation Processes in the Environment. Dubrovnik, Croatia.
Dr A. Sabljic, Institute Boskovic, POB 1016, HR-10011 Zagreb, Croatia

Organic synthesis

28 June–2 July
12th International Conference on Organic Synthesis. Venice, Italy.
Depha Congress SRL, Viale Majno 21, 20122 Milano, Italy. Tel.: +39 (2) 76008190; Fax: +39 (2) 782400; E-mail: dephadue@mbox.vol.it

Chemistry in Africa

6–10 July
7th International Chemistry Conference in Africa (7th ICCA). Durban, South Africa.
The Secretary, 7th ICC & 34th SACI Convention, Department of Chemistry & Applied Chemistry, University of Natal, Durban 4041, South Africa. Tel.: +27 (31) 3603090. Fax: +27 (31) 2603091; E-mail: 7icca@che.und.ac.za

Macromolecules

13–17July
37th International Conference on Macromolecules, Gold Coast, Australia.
Prof. R.G. Gilbert, School of Chemistry, F11, Sydney University Polymer Center, University of Sydney, New South Wales 20006, Australia. Tel.: +61 (2) 351 3366; Fax: +61 (2) 351 3329;
E-mail: gilbert@chem.usyd.edu.au

20–23 July
18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.
P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, CZ-162 06 Prague 6, Czech Republic. Tel.: +420 (2) 360341; Fax: +420 (2) 367981;
E-mail: sympo@imc.cas.cz

Chemical thermodynamics

26 July–1 August
15th International Conference on Chemical Thermodynamics. Porto, Portugal.
Prof. M.A.V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal.

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (171) 4378656; Fax: +44 (171) 7341227.

Novel aromatic compounds

2–7 August
9th International Symposium on Novel Aromatic Compounds, Hong Kong.
Prof. H.N.C. Wong, Chairman, Local Organizing Committe, 9th International Symposium on Novel Aromatic Compounds, Department of Chemistry, Chinese University of Hong Kong, Shatin, New Territories, Hong Kong.

Solubility phenomena

5–8 August
8th International Symposium on Solubility Phenomena. Niigata, Japan.
Prof. H. Akaiwa, Faculty of Engineering, Gunma University, Kiryu 376, Japan.

Chemical education

9–14 August
15th International Conference on Chemical Education: Chemistry and Global Environmental Change. Cairo, Egypt.
Prof. Saad S.M. Hassan, Department of Chemistry, Faculty of Science, Ain Shams University, Cairo, Egypt.

Physical organic chemistry

16–21 August
14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.
Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento di Química, 88040-900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy. Tel.: +39 (55) 2757549. Fax: +39 (55) 2757555.

Medicinal chemistry

6–10 September
25th International Symposium on Medicinal Chemistry. Edinburgh, Scotland.
Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (0)171 437 8656; Fax: +44 (0)171 734 1227.

Natural products

11–16 October
21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.
Prof. Xibai Qiu, Secretariat of ISCNP-21, c/o Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: +86 (10) 62568157 or 62564020; Fax: +86 (10) 62568157; E-mail: qiuxb@infoc.3.icas.ac.cn

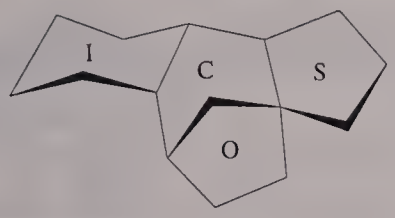
2000

Macromolecules

9–14 July
MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.
Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90-363 Lodz, Poland. Tel.: +48 (42) 819815; Fax: +48 (42) 847126.

Biotechnology

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.



ICOS 12
June 28 - July 2, 1998
Venice, Italy

Thieme Publishers and IUPAC in collaboration with the editors of
SYNTHESIS · SYNLETT · HOUBEN-WEYL · SCIENCE OF SYNTHESIS
announce the 1998

Thieme-IUPAC Prize in Synthetic Organic Chemistry

sponsored by
Georg Thieme Verlag Stuttgart · New York

The **Thieme-IUPAC Prize** is presented every two years on the occasion of the International Union of Pure and Applied Chemistry – International Conference on Organic Synthesis (IUPAC-ICOS). The 1998 ICOS will be held in Venice, Italy, on June 28 – July 2.

Prize DM 10 000

The prize is awarded to a scientist **under 40 years of age** (as of January 1 of the year in which the prize is awarded) whose research has had a major impact in synthetic organic chemistry.

The Thieme-IUPAC Prize has been awarded to Stuart L. Schreiber (Harvard) in 1992, Paul Knochel (Marburg) in 1994 and Eric N. Jacobsen (Harvard) in 1996.

Call for Nominations
(deadline December 12, 1997)

The prize will be awarded on the basis of scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials.
Proposals must be accompanied by a biographical sketch of the nominee, a list of the candidate's ten most significant publications, and a statement of how the candidate's research has had a major impact on the field of synthetic organic chemistry.

Nomination materials **(8 copies)** should be submitted by December 12, 1997 to Lindsey Sturdy, Georg Thieme Verlag, Rüdigerstraße 14, D-70469 Stuttgart, Germany. Telephone +49 (711) 8931 310; Fax +49 (711) 8931 311; e-mail lindsey.sturdy@thieme.de.

Thieme

Georg Thieme Verlag
P. O. Box 30 11 20
D-70451 Stuttgart · Germany

b
Blackwell Science

Osney Mead,
Oxford OX2 0EL,
UK

Telephone
(01865) 206206

Fax
(01865) 206096

Compendium of Chemical Terminology

The Gold Book

Second Edition

IUPAC

Edited by A D McNaught and A Wilkinson

This new second edition of the IUPAC '*Gold Book*' represents a very substantial enhancement of the first.

In the 10 years since the first edition, IUPAC has revised and updated most of the original definitions, and has produced new glossaries of terms in many areas of chemistry not previously covered. Around 7000 entries cover all the traditional areas of chemistry and also growing fields such as stereochemistry, photochemistry, organic class names, atmospheric chemistry, catalysis, biotechnology, chromatography, toxicology and bioanalytic chemistry. The resulting compendium, like the first edition, contains only definitions approved by international concensus, and thus can be regarded as truly authoritative.

- **the only truly authoritative reference available - now fully updated and significantly expanded**
- **an essential reference resource for chemists everywhere**

August 1997 . 464 pages . Illustrated . ISBN 0865426848
Paperback £39.50/US$49.50
IUPAC Members discount price £23.70/US$29.70

Order Form

☐ Please send me _____copy/ies of ***McNaught: Compendium of Chemical Terminology*** at the IUPAC members price of £23.70/US$29.70 plus £2.50/US$5.00 postage and packing

☐ Please send me _____copy/ies of ***McNaught: Compendium of Chemical Terminology*** @ £39.50/US$49.50 plus £2.50/US$5.00 postage and packing

☐ I attach a cheque (made payable to Marston Book Services) for the sum of £_____/US$_____

☐ Please charge my AMEX/Diners Card/Eurocard/Mastercard/VISA

card number | | | | | | | | | | | | | | | | expiry date_____

with the sum of £___ US$___ Signature_____ Date_____

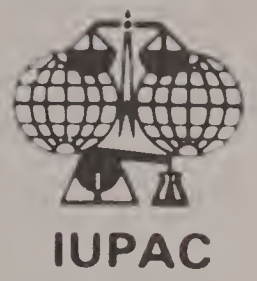
Name_____

Address_____

_____

Please return to Anna Rivers at the address opposite:

International Union of Pure and Applied Chemistry (IUPAC)



President: A. E. FISCHLI (*Switzerland*)
Vice-President: J. JORTNER (*Israel*)
Secretary-General: E. D. BECKER (*USA*)
Treasurer: J. M. WARD (*UK*)

IUPAC Secretariat

PO Box 13757, Research Triangle Park, NC 27709-3757, USA. Tel.: +1 (919) 485 8700. Fax +1 (919) 485 8706. E-mail: johnwjost@compuserve.com

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 39 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Neue Schweizerisches Chemische Gesellschaft **(Switzerland)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1997, Vol. 19, No. 5 (September)

151 Relocation of the IUPAC Secretariat

152 The President's Report
Albert E. Fischli

156 Secretary General's Report
Edwin D. Becker

158 Biennial Report of the Treasurer and Finance Committee
J.W. Ward

160 Treasurer's Review 1991–1997
J.W. Ward

161 Relocation of IUPAC Archival Material

163 Recent Reports

169 PAC Review

170 News

173 New Publication

173 Conferences

174 Conference Calendar

Information on this magazine can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

b
Blackwell Science

0193-6484(199709)19:5;1-P

Printed in Great Britain by Alden, Oxford, Didcot & Northampton

ISSN 0193-6484

New names and addresses pull-out

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

1997, Vol. 19, No. 6 (November)

Blackwell Science

Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

PRODUCTION EDITOR: Howard Waller

All correspondence to be addressed to The Editor, Chemistry International, IUPAC Secretariat, PO Box 13757, Research Triangle Park, NC 27709-3757, USA. Telephone: +1 (919) 485 8700. Fax: +1 (919) 485 8706. E-mail: johnwjost@compuserve.com and http://chemistry.rsc.org/rsc/iupac.htm

Editorial Advisory Board

Chairman:	E. D. BECKER	*Secretary General*		
	E. BUNCEL	*CHEMRAWN Committee*		
	A. SMITH	*Committee on Chemistry and Industry*		
	D. H. M. BOWEN	*Committee on Printed and Electronic Publications*		
	I. M. MILLS	*Interdivisional Committee on Nomenclature and Symbols*		
	M. E. PESTANA	*Committee on Teaching of Chemistry*		
			G. SOMSEN	*Division I*
			G. J. LEIGH	*Division II*
			G. SAVELLI	*Division III*
			A. ABE	*Division IV*
			F. INGMAN	*Division V*
			T. R. ROBERTS	*Division VI*
			(To be appointed)	*Division VII*
Acting Secretary:	J.W. JOST	*Executive Director*		

Subscriptions

Six issues of *Chemistry International* will be published bimonthly in 1997 (one volume per annum) in January, March, May, July, September and November. The 1997 subscription rate including postage is GBP 75.00 (UK and overseas except North America) or USD 116.00 (US and Canada). The individua! subscription rate is GBP 29.00 (UK and overseas except North America) or USD 42.00 (US and Canada). Microfiche subscriptions are available simultaneously with the printed edition, and microfilm at the end of the subscription year. Subscription orders may be placed directly with IUPAC's official publisher, Blackwell Science Ltd, PO Box 88, Oxford, UK; E-mail: journals.cs@blacksci.co.uk. Information on this journal can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Advertising. Enquiries should be sent to the Advertising Manager, Blackwell Science Ltd, Osney Mead, Oxford OX2 0EL, UK. Telephone: +44 (0) 1865 206206, Telex 83355 Medbok G, Fax +44 (0)1865 721205.

Despatch. The news magazine is despatched within Europe by surface mail, to other continents by various forms of air-speeded delivery: to the US* by air freight for forwarding by periodicals post, to India by air freight for guaranteeed local delivery, and to all other countries by Accelerated Surface Post.

Reproduction of Articles

Unless there is a footnote to the contrary, reproduction or translation of articles in this issue is encouraged, provided that it is accompanied by a reference to the original in *Chemistry International*. The Blackwell Science logo is a trade mark of Blackwell Science Ltd registered at the United Kingdom Trade Marks Registry.
This journal is included in the ADONIS service, whereby copies of individual articles can be printed out from compact discs (CD-ROM) on demand.

*Periodicals postage paid at Rahway, NJ. Post Master, send address changes to *Chemistry International*, c/o Mercury Airfreight International Inc., 2323 Randolf Avenue, Avenel, NJ 07001, USA.

Front cover: Dr Mo Williams receives a silver salver from Prof. Albert Fischli in recognition of 29 years' service to IUPAC (see page 179).

Secretary General's Column

Edwin D. Becker

In this month's column I would like to comment on the 39th General Assembly, held in Geneva, Switzerland, 23–30 August 1997, and to report some of the major actions by the Bureau and Council. In my opinion, this was a very successful meeting, in which about 670 chemists participated, primarily in dozens of meetings of small groups—commissions, committees, working parties and task forces. The enormous amount of scientific work done during the long hours of each day's meetings covers a range of subjects much too diverse to be described here, but this dedicated effort on the part of many volunteers forms the core of IUPAC's accomplishments.

The venue of the General Assembly was the University of Geneva, where we found excellent facilities and superb services provided by the local organizing committee, under the chairmanship of Prof. Jacques Weber. Most of the detailed arrangements and services fell to Mme. Nathalie Girard and her staff, who not only met all our needs but anticipated virtually all of them to provide a very smoothly running meeting.

Scientific Policy and Management of Projects. Looming as background to the entire General Assembly was the issue of restructuring the Union and updating our mission and goals to face the world-wide challenges of the modern world of chemistry. In my column in the July issue of *Chemistry International*, I summarized proposals to develop specific long-range goals for IUPAC, to introduce more flexibility into the appointment and operation of commissions and working parties, and to emphasize a project-driven system. The Strategy Development and Implementation Committee (SDIC) is addressing these issues, and the General Assembly provided an ideal forum for everyone, ranging from individual Commission Members to Division Presidents, to express views and provide valuable input to the SDIC's planning process. The SDIC will meet in early 1998 to develop specific proposals, and I will keep readers of *Chemistry International* informed of the results.

Meanwhile, at Geneva a number of discussions in

both the Bureau and Council recognized the importance of the SDIC's task. While voting to extend the term of all Commissions until the end of 1999 (except for one Commission whose responsibilities have been taken over by a Technical Committee of the International Standards Organization), Council made clear its concerns about the need for sharper focus of the Commissions' activities when it approved a resolution introduced by the UK, 'Council urges Division Committees to continue to propose topics of importance for study and report by their Commissions. Commission programmes should be carefully controlled and/or reduced by at least 25% over the next two years so that high priority programmes may be completed more expeditiously and efficiently in future'. The SDIC and the Executive Committee will determine how best to implement this requirement.

Elections. Council elected Dr Alan Hayes, outgoing Chairman of the CHEMRAWN Committee, as Vice-President for the next biennium and President in 2000–2001, and it elected Prof. John Ward to complete a final two-year term as Treasurer. Six vacancies on the Bureau were filled by election of Dr E.P. Przybylowicz and Prof. G. Somsen and re-election of Profs. E.J. Grzywa, J.W. Lorimer, L.K. Sydnes and C.-H. Zhang for a second term. The Bureau elected Dr. Przybylowicz and Prof. H. Ohtaki to fill vacancies on the Executive Committee. A complete list of Bureau Members and of Officers of all IUPAC bodies for 1998-99 is included with this issue of *Chemistry International*, pages 197–212.

Individual Member Programmes. During the last two years the Affiliate Membership Programme has been analyzed by an *ad hoc* committee set up by the Bureau under the Chairmanship of Prof. Jack Lorimer. Two years ago the AMP was thought to be a financial drain on the Union, but changes in operational policies have reduced costs, and future activities centred at the new Secretariat are expected to emphasize electronic communications,

with further cost reductions. Council approved the Lorimer Committee's recommendation to continue the AMP for the next biennium, during which further efforts will be made to expand membership and revitalize the Programme.

The Lorimer Committee made a second important recommendation, also approved by Council, to establish an IUPAC Fellows Programme, which will be open to all persons who have completed service on any IUPAC body. This Programme will recognize the service to IUPAC by these individuals, will facilitate their continuing involvement with the Union, and will gradually establish a large cadre of people who can provide a source of ideas and expertise for future IUPAC projects. Policies and procedures for implementing the Fellows Programme will be developed and implemented during the coming months.

Membership of the Union. Council approved the admission of National Adhering Organizations (NAOs) from Yugoslavia, Puerto Rico and Pakistan. Yugoslavia (representing chemists in Serbia and Montenegro) constituted a readmission, while Pakistan and Puerto Rico were previously Observer Countries. There are now 42 NAOs in IUPAC.

Council established a category of Provisional Membership to permit the Bureau or Executive Committee to act provisionally on applications from potential NAOs between Council meetings. Council also agreed that individual experts from non-adhering countries may serve provisionally on IUPAC Commissions and Committees.

Names of Elements 101 to 109. As usual, Council was called on to ratify all recommendations for nomenclature and symbols approved on its behalf by the Interdivisional Committee on Nomenclature and Symbols. Because of the controversy surrounding the names of the transfermium elements, a separate vote was taken on this document and resulted in overwhelming approval of the revised recommendation by the Commission on Nomenclature of Inorganic Chemistry, which will appear in the December 1997 issue of *Pure and Applied Chemistry*. The recommended names and symbols, as announced previously (*Chemistry International* 1997, **19**, 68–69), are:

Element	Name	Symbol
101	Mendelevium	Md
102	Nobelium	No
103	Lawrencium	Lr
104	Rutherfordium	Rf
105	Dubnium	Db
106	Seaborgium	Sg
107	Bohrium	Bh
108	Hassium	Hs
109	Meitnerium	Mt

NAOs and national chemical societies are being urged to adopt these recommendations, and that has been done in at least one large country. The Nomenclature Committee of the American Chemical Society, which met soon after the IUPAC General Assembly, endorsed all the names, which will be used henceforth in ACS publications.

Finances. Council accepted the Treasurer's recommended budget for 1998–99, along with an increase in national subscriptions of 3% each year to maintain approximately constant real income in the face of expected inflation.

Tribute to Mo Williams. Council paid tribute to Dr Mo (Maurice) Williams, who retired in April after 29 years of service as Executive Secretary to IUPAC. He has remained in an advisory capacity for the last six months. President Fischli presented Dr Williams with a silver salver inscribed with the signatures of the 15 IUPAC Presidents under whom he served (see page 179).

Future Congresses and General Assemblies. Council gave final approval to Berlin as the site of the 40th General Assembly (7–14 August 1999) and 37th Congress (14–19 August 1999). The 40th General Assembly will be held at the Freie University of Berlin, and the 37th Congress at the International Congress Center in Berlin. Council also accepted the proposal of the Australian NAO to hold the 38th Congress and 41st General Assembly in Brisbane, Australia, in 2001. The 38th Congress is provisionally scheduled for 1–6/7 July 2001 at the Brisbane Convention Centre, and the 41st General Assembly for 7–14 July 2001 at the University of Queensland, Brisbane. Final approval is expected to be given in two years, when detailed plans have been formulated.

Prof. Heindirck tom Dieck, Organizer of the 1999 IUPAC Congress

Presentation to Dr Mo Williams

During the 39th Council meeting at Geneva (29–30 August 1997), IUPAC's President, Prof. Albert Fischli, made a presentation to Dr Mo (Maurice) Williams, who retired in April after 29 years as Executive Secretary of the Union:

'I have the privilege and the very personal pleasure to say goodbye to Dr Williams, to wish him all the best for his retirement, and to welcome him as a personal advisor to our new Executive Director, Dr John Jost, until the end of October.

'Despite his Welsh name and the Welsh propensity, not to use one word where six will do, Mo was born and raised in Birmingham, UK. He graduated BSc in chemistry at Birmingham University in 1953, and went on to do a PhD in Prof. Ron Belcher's eminent School of Analytical Chemistry under the joint supervision of Belcher and (then) Dr Tom West.

'Leaving Birmingham University in 1956, he spent two years in ICI Metals Division's Research and Development Department, which was much concerned at that time with the analysis of new metals like titanium, zirconium, and beryllium, and their alloys.

'In 1959 he moved to become lecturer in analytical chemistry at Birmingham College of Advanced Technology, which is now the University of Aston. While there, he became Editor-in-chief of Mr Robert Maxwell's international analytical chemistry journal *Talanta* (Pergamon Press). His qualities were recognized by Maxwell, who offered him the post of managing editor/learned journals at Oxford, which he accepted from the start of 1966.

'When he was offered the opportunity to become the first professional IUPAC Executive Secretary in April 1968, he accepted provided that the office could be in Oxford. By the way, the suggestion came through Belcher and West, both of whom served as Presidents of the Analytical Division of IUPAC, and Tom West later on then also as Secretary General.

'That is how we first saw him, and now 29 years later one can say that he is really "Mr. IUPAC".

'Outside IUPAC, he has been an engaged contributor to the administration of sport. He was County President of the Oxfordshire and North Buckinghamshire Amateur Swimming Association in 1984.

'As we all know, he is a keen golfer and he looks forward to devoting much more time to it in his retirement, along with his wife, also a keen golfer.

'He has always been a keen and vocal supporter of Aston Villa Football Club and, if at this General Assembly Mo's smile seems somewhat strained, it is probably because Aston Villa is at present at the bottom of the British Premier League.

'I have the pleasure to hand over to you Mo, a small present, a silver salver with the signatures of all the 15 Presidents of IUPAC under whom you served.

'Let me also express the thanks of IUPAC to Mrs Ulrike Inglis who came to the IUPAC Secretariat at Oxford in 1976, to Mrs Erica Sheppard who joined us in 1977, and to Mrs Sandra Hornblow who started work with the Union in 1989. IUPAC would like to express its appreciation for all that you have done for the Union, and we wish you all the best for your future.'

In his reply, Dr Williams said that, despite the inevitable ups and downs, overall the 29 years had been an exciting time and a privilege to serve as the Union's Executive Secretary. In addition to working under 15 Presidents, there had been six Secretaries General and five Treasurers, and he has made countless friends throughout the world. The growth in work for the Secretariat was reflected in the fact that only two Commission reports were published in *Pure and Applied Chemistry* during 1968, but there would be over 50 in 1997. Fortunately, he had been supported throughout by excellent colleagues: besides the three secretaries present at

Mo Williams receives a silver salver from Prof. Albert Fischli

Geneva, two others had remained at Oxford, and there had been exceptional backing from Miss Ann Troughton (Assistant Executive Secretary) for 20 years and from Dr Mike Freemantle (Information Officer/Affiliate Affairs Secretary) for nine years. Dr Williams offered his best wishes to Dr Jost for the wider development of electronic services at the new Secretariat in Research Triangle Park, North Carolina.

The presentation to the IUPAC secretaries by Prof. Fischli

36th IUPAC Congress

17–22 August 1997, Geneva, Switzerland

The 36th IUPAC Congress was a success by many measures. Attendance was 1251 from 59 countries; there were more than 900 presentations: 9 plenary, 40 keynote, 40 invited, 30 short contributions and 832 posters; one-third of the participants were under 30 years old. Fifty-six countries were represented among the poster presenters. The following table indicates the international character of both the participants and the presentations at this Congress.

The nineteen countries in this table represent all those countries that had ten or more participants, 88% of the total. These nineteen countries also had 83% of the posters. All of the major geographic areas of the world are well represented except sub-Saharan Africa.

Prof. Jacques Weber opens the Congress

This Congress is the first to be guided to a great extent by the report of Prof. G. Modena and Prof. J. Jortner, presented to the 65th Bureau, 17–18 September 1994. This report proposed that IUPAC should act to make the IUPAC Congress a central international event by fulfilling the following goals:

Country	Number of Participants	Number of Posters
Switzerland	502	201
Turkey	58	85
Japan	79	57
Russia	25	40
Poland	32	37
Germany	96	34
Egypt	19	30
China	21	29
Taiwan	29	26
USA	58	25
Macedonia	15	24
Iran	21	23
France	41	21
Canada	17	14
UK	29	13
Ukraine	10	13
Italy	20	8
Netherlands	16	8
Israel	13	5
Totals	1101	693

1 To present the most outstanding relevant developments in modern chemistry
2 To inspire high standards of excellence in pure and applied chemistry research
3 To attract outstanding scientists to present central lectures on modern chemical research
4 To inspire the young generation of chemists in developed and developing countries

While the time from the adoption of these principles to the organization of the 36th Congress was too short for full implementation, this Congress fulfilled in large part the aim of the report to improve the quality and impact of IUPAC Congresses. In particular the large participation by younger chemists, the broad international character of both the attendees and the presentations, and the emphasis on topics at the *Frontiers of Chemistry*, are all in the spirit of the proposals for the revitalization of the IUPAC Congresses made by Profs Modena and Jortner.

The opening Plenary lecture by Prof. Peter Schultz of the University of California, Berkeley, set the tone by demonstrating that chemistry is at the heart of advances in modern biology and materials science. This lecture also gave a vivid demonstration of ways in which understanding gained in one area can be applied to what may seem a quite unrelated subject. In this case, Prof. Schultz showed that the attempt to understand how the human antibody system solves the problem of recognizing an essentially infinite number of possible antigens led to new insights in the development of catalysts and materials.

Prof. Peter Schultz

The Plenary lecture by Prof. Paul J. Crutzen of the Max Planck Institute for Chemistry, Mainz, moved the discussion from the chemistry of the inside of the human body to the effects of human activity on global climate. His review showed the major consequences for global climate and the inhabitants of the earth, of the complex interactions of simple molecules and ions at relatively low concentrations. Prof. Crutzen also described new and unexpected interactions of human activities and the chemistry of the atmosphere.

Prof. Paul J. Crutzen

The 3rd Plenary lecture, by Prof. Richard N. Zare of Stanford University, moved back from the examination of chemistry at the global scale to the investigation of single molecules. This lecture demonstrated the combination of a technique from the frontiers of physical chemistry, femtosecond laser spectroscopy, with vesicles conceptually related to the 'containers' used by biological systems to isolate and transport molecules, to isolate and examine individual molecules.

Prof. Richard N. Zare

The 4th Plenary lecture by Prof. J. Nüesch, President of the ETH-Zürich, addressed the issue of ethics and sustainability in chemistry. As had been pointed out by Prof. Crutzen, human activities can have a significant effect on the global ecosystem. Prof. Nüesch discussed the ethical demands in chemistry, which he described as being especially important because of the ability of

chemical technology to affect humanity for both good and ill. This can lead to the common ethical dilemma of our time, the need to balance the improvement of living standards through the application of technology while at the same time considering the possible effects of that technology on the global environment.

Prof. Dieter Seebach of the ETH-Zürich reviewed the changing focus of classical organic synthesis into areas related to molecules of biological interest. His theme was the continuity of the science as it moves to new frontiers. He reminded his audience that while the focus may change, the underlying nature of the synthetic enterprise remains the same, namely the development of synthetic techniques that allow control of the chemistry leading to new kinds of molecular structures.

Prof. Dieter Seebach

Prof. Olivier Kahn reviewed the field of molecular magnetism, a field that combines aspects of organic, inorganic, organometallic, and physical chemistry as well as materials science. His review introduced the concept of the magnetic brick, a building block which can be used to construct new one-, two- and three-dimensional species. This lecture again demonstrated the application of the classical concepts of chemistry leading to developments at the frontiers of traditional discipline boundaries.

Prof. Olivier Kahn

Prof. Gerhard Ertl of the Fritz–Haber Institute of the Max-Planck Gesellschaft in Berlin reviewed new surface analytical techniques that have led to an understanding of processes at a microscopic scale. In particular, those microscopic level processes that control processes at a macroscopic level. His review connected new understanding of the interactions of simple molecules at metal surfaces with the large-scale processes occurring in industrial heterogeneous catalysis.

Prof. Gerhard Ertl

Prof. Gilbert Balavoine of the Laboratoire de Chimie de Coordination, CNRS, Toulouse discussed the major rôle played by chemistry in society—a rôle that is not matched by an understanding on the part of society of the use of the technology developed by the chemical sciences. This lecture returned to the theme of the earlier lectures by Profs Crutzen and Nüesch regarding the ethical and social implications of the applications of chemical technology.

Prof. Gilbert Balavoine

The final Plenary Lecture by Prof. C. Weissmann of the University Zürich discussed a particular application of chemistry at the frontiers of molecular biology. A prion is believed to cause both scrapie in sheep and bovine spongiform encephalopathy (BSE). The investigation of the transmission and propagation of this prion demonstrated the use of chemical knowledge,

developed over the past decades, to investigate a problem that is usually viewed as a biological problem. (The award of the Nobel Prize for Medicine to Prof. Stanley B. Prusiner for the discovery of prions demonstrates the timeliness of this topic.)

It is impossible to discuss here the dozens of other keynote and invited lectures at the Congress, much less the hundreds of posters. The organizers of the Congress, Prof. J. Weber, Prof. F. Diederich and Prof. A. von Zelewsky, are to be congratulated on assembling a group of Plenary Lecturers who provided such an exciting and informative overview of the future of the chemical sciences.

I would like to acknowledge the fine photographs by Karin Hedinger.

John W. Jost
Executive Director

Meeting of the Chemical Society Presidents

On Saturday 23 August 1997—sandwiched between the IUPAC Congress and the General Assembly—the New Swiss Chemical Society organized an international meeting at the Hotel Noga Hilton, Geneva, to which the presidents of all chemical societies worldwide were invited. Over 50 attended to hear two top-level representatives of the Swiss chemical industry speak on the theme: 'The chemist, facing the structural changes in the chemical industry'. An edited version of a discussion-provoking presentation by Dr Hans Kindler, Member of the Executive Committee of Novartis, Basel, is reproduced here.

Dr Hans Kindler

The significance and the image of the chemical industry and the position, the mission and the professional perspectives of the chemist have experienced significant changes over time. There have been continual changes from the medieval alchemist, a magician searching for gold and immortality, to the scientists of the early 19th century creating the modern sciences and striving to understand and control the elements and the processes of life, to the chemists of a hundred years ago who produced the first manmade dyestuffs on a large scale. The beginning of medicinal chemistry in the 1920s, the increasing knowledge and understanding of chemical reactions and the new material sciences brought further changes. The increasing knowledge about biological processes, the growing relevance of biochemistry and the rapid developments in the field of genetics, in data management and information technology have more recently had a remarkable impact on the role of the chemist.

In all these different eras there was a common feature: for people who are not familiar with the profession there have always been somewhat unclear and sometimes unrealistic notions about the activities, possibilities, limitations and the power of chemists.

The working environment for the chemist, the mission, and working conditions, have also experienced important changes during the past few decades. In the first half of this century an industrial chemist worked either in a research laboratory at the bench or in chemical production. In either case the chemist worked in isolation with little communication and almost no flow of information across the organization. The business was technology driven, chemical research and manufacturing were the core competencies and production had a preferred central position.

Since the 1950s the pharmaceutical/chemical industry has become more and more market driven. New and innovative products have had to be developed and

manufactured to satisfy customers. A good integration of R&D projects in business strategy has become important to manage the innovation process successfully.

Over the same period, understanding of biological and biochemical processes has increased at a rapid pace, leading to a stronger influence of the biosciences in the discovery and development process. In manufacturing, efforts to improve the production processes have been extended from optimizing the cost of production to improving safety and ecology parameters at the same time. All these trends have led away from the working approach of the isolated chemist to an interdisciplinary working environment, to the team approach and an open communication across boundaries of departments, disciplines and locations.

For the chemist these developments mean above all that there is no special status; the chemist has to be able and willing to work in interdisciplinary teams. There are two major areas through which the chemist in industry can proceed and contribute value to the company:

- In the area of life sciences the chemist's knowledge is integrated with that of biologists and other specialists in medicine or animal and plant sciences;
- In material sciences there are many opportunities and challenges for innovation. There is a need for new materials such as composites, ceramics and catalysts for manufacturing, as well as for new analytical methods, chemical sensors and optoelectronic devices.

Against this background of change we ask ourselves what will be the impact on the chemist's future role.

Changes in the economic environment

The economic environment of the chemical industry is influenced primarily through the globalization of markets and increasing competitive pressures. Through networks of trade and information all major products and services are today offered worldwide and the competitive edge of many products is determined by the ability to differentiate them in performance or price.

Traditional home markets which previously determined the product range no longer exist. Home markets have the same rules as global markets.This also means that preferred locations for marketing organizations and technical operations are increasingly determined by strategic factors, the availability of resources, the social and legal environment and the proximity to customers.

Players in global markets have to adjust their structures and locations and must refocus their activities in view of their competitive advantage. This is leading to an increasing concentration of the industry through mergers and acquisitions. Companies have to exploit their synergy potential through management effectiveness, rationalization and focusing on core competencies. Outsourced segments offer many opportunities for small, highly specialized or start-up companies. Additionally, we observe a dramatic increase in innovation costs and greater expectations and pressures of the financial community.

Another source of change, particularly affecting the pharmaceutical industry, is the 'power shift' of customers. Traditionally the medical doctor decided and prescribed the therapy and the medication for his patients. The decision power is now shifting more and more towards the payer, the health insurance companies and the patient. This shift influences the marketing strategies, organizational structures, product range and supply concept of the pharmaceutical industry.

The chemical industry's resources are increasingly focused on segments with high value-added potential and on product innovation and improvement.The value-added segments are increasingly shifting from the producer to the creator of ideas and innovations. A strong process and product innovation effort is therefore the crucial factor for long-term success in the high added-value segment of any business. Consequently the chemical industry's R&D activities are increasing in absolute terms as well as in percentage of sales.

Changes in science and technology

Developments in science and technology are among the most striking and highly visible changes taking place in our industry. There have never been so many people with such a high level of knowledge and never was communication of results and data so thorough and so easy. Information technology and computer power facilitates most tasks of the chemist and enables progress in areas such as gene technology. As a result, the disciplines of chemistry, biology and medicine are moving closer together.

Molecular biology is broadening the scope of the tools available in life sciences. These are complementing, not replacing, the range of currently available methods and products in healthcare, plant breeding and crop protection. The full impact of methods such as somatic gene therapy and xenotransplantation is not foreseeable yet; however, we have to be prepared to stay at the forefront of such developments.

New technologies are also developing in the non-biological sciences. In material sciences, new lightweight materials with improved mechanical and heat stability properties are being developed. New supramolecular structures are being investigated which exhibit unusual optical, optoelectronic and magnetic properties useful for data storage and other electronic or optical devices. Research in catalysis, especially in stereoselective reactions, has made great progress and opens new possibilities for ecologically improved manufacturing

processes. New territory is also being explored in the research of energy storage and molecular batteries, in sensor technology and analytical/diagnostic tools.

Obvious examples of multidisciplinary techniques are the new approaches in synthesis and testing large libraries of compounds, in computational and combinatorial chemistry and high throughput screening.

Changes in the social environment

A recent study by the German Institute for Economic Research (DIW) has confirmed a clear pattern of internationalization of the industry: sites for industrial manufacturing follow the customer. Sooner or later R&D follows. As well as economic parameters, legal and social factors influence the selection of production and R&D sites. The social changes taking place in Europe today are characterized by reluctance to accept the activities of the chemical industry, including genetic engineering, the necessity to experiment with living organisms and the need for full intellectual property protection.

Ongoing changes in legislation should also be mentioned. Government activities and industry efforts should be complementary. Initiatives such as those being launched in Switzerland to forbid the use of some technologies are restricting development in the country. An attractive country for an innovative industry has to provide an innovation friendly environment with a positive attitude towards new technologies. This includes practicable legislation in the areas of ecology, animal rights, gene technology and which permits for the construction and operation of pilot plants.

Consequences for the position of the chemist

Economic environment

Among the economic changes taking place in our business it is the globalization of markets which will have the most significant impact on the situation of the chemist. Participating in new attractive markets means that some production and R&D sites will be transferred to new sites and locations. The industry needs chemists with leadership qualities who are flexible and prepared to move to new assignments, activities and geographical areas—people with a sound basic knowledge of their professional field and the ability to see the entire picture of the business.

The ongoing structural changes in the pharmaceutical/chemical industry are not only aimed at increasing shareholder value, but are essential to realize synergies, to achieve a greater presence in the market place and to reach a critical mass for innovation potential. Chemists and other scientists in this R&D environment have to understand the driving forces of the markets and the dynamics of the business. They must be capable of translating market needs into R&D programmes and projects and they must have the ability to explain what they are doing in generally understandable terms.

While some big companies, for example the automotive industry in the USA, reduce their size and structures, many existing positions are substituted. Several activities and services, production of parts and manufacturing of intermediates for example, are outsourced, which creates new opportunities for start-up companies, as can be demonstrated by the figures of the US industry. During the period 1993–95 the large US concerns eliminated 3.6 million jobs; at the same time, 5 million new positions were created by small and start-up companies. The chemical industry is subject to the same changes and for this process needs scientists with entrepreneurial qualities and economic thinking.

Social factors

As a result of unclear notions about the profession of the chemist, reluctance to accept scientific progress—even fear among the public—and the present tight job situation in the European chemical industry, the number of chemistry students in Europe has significantly declined in recent years. As a consequence public funds for research and teaching in chemistry are also decreasing (universities, national funds). We have to make real efforts to maintain the high scientific standards that makes Switzerland an attractive country for the chemical/pharmaceutical industry. Many respectable colleagues predict a significantly increased requirement for chemists over the next 5–10 years.

Science and technologies

New technologies, above all information technology and molecular biology and their application in genetic engineering, have changed the working environment of the industrial chemist. The new technologies are complementary with traditional chemistry and provide new challenges and opportunities for chemists in the chemical-biological direction as well as in the area of chemical engineering, production and material sciences.

Information technology has changed the working environment of many professions, including chemists. Handling literature and patent searches, managing data, accessing data banks, searching and designing of new active entities and process control, are a few important applications, requiring knowledge and command of electronic tools.

The increasing complexity of the subjects requires a working approach with interdisciplinary teams. The chemical industry will therefore need chemists who are able to manage and to contribute to interdisciplinary teams and processes in the areas of chemistry, engi-

neering and in biosciences. Chemists generally have good access to other disciplines and to an interdisciplinary working environment. They have to be trained even more to approach tasks and problems as team players.

In a recent survey by the New Swiss Chemical Society several managers confirmed these statements and emphasized that medium-sized and start-up biotechnology research companies will employ increasing numbers of chemists, because the majority of future drugs will be synthetic products. The exact figures for open positions for chemists in the chemical industry for the next few years are not known; the New Swiss Chemical Society has initiated a survey to study the future need for chemists in the Swiss industry. It is important to note that the new technologies may cause a restructuring and refocusing of industrial functions and sectors, but they cause a substitution rather than a reduction in positions for scientists.

The education and training of the new generation of chemists has to be adapted to the requirements of a sound knowledge of basic chemistry, an understanding of the areas of application, the management and working habit of interdisciplinary teams and an understanding of basic economic principles.

Education and universities

In the course of the 'Third International Mathematics and Science Study' about half a million students aged 14 from 28 countries were tested in mathematics and natural sciences and their results were ranked. The Swiss students ranked eighth in mathematics, but only 18 in natural sciences. This is an alarming result, whatever the reasons may be, large classes, few hours of teaching natural sciences, lack of interest of the teachers or lack of learning pressure. The Swiss authorities, the Department of Education, the Cantons and their bodies should take actions for improving this situation.

The public education system, particularly at university level, is of fundamental importance for preparing chemists for their industry position. At universities and institutes of technology teaching and research belong close together. Unfortunately some professors focus their entire interest in their research and consider teaching a burden. Let me state very clearly that the chemical industry considers teaching as the primary mission of universities. High quality research is a good and sound base for excellence in teaching. We expect chemists to receive a first class, diversified education which prepares them for various positions in industry and gives them a high degree of flexibility in their choice of positions. Universities have to get away from the idea of preparing chemists exclusively for their professional position as researchers. Teaching schedules should also include basics in law, economics, communication and social issues. These topics should be integrated into the regular schedule for students without extending the present time for studying chemistry.

Conclusions

In conclusion I am convinced that the position and the professional profile of the chemist in today's chemical industry is subject to an evolution, as markets, industry structures and technologies are changing. The requirement for well-educated, versatile and flexible chemists in different business areas is high. Future scientists will need the ability to work in interdisciplinary teams and have well-trained social and communication skills. Familiarity with the applications of information technology and the potential of processes in biotechnology and engineering sciences is essential.

Interest and enthusiasm for science subjects are generated at primary and high school level. The situation in many countries and certainly in Switzerland is mediocre and needs to be improved. It is an important task for the professional organizations and the chemical industry to provide open information about the attractiveness and beneficial contributions of the profession and the future need for chemists.

The chemical industry will continue to engage in dialogues with the public, with authorities and schools, in order to improve the image and knowledge about the merits of the industry and the profession of the chemist. The industry will also continue to support the education of chemists at educational institutions by common projects and cooperations, by sponsoring scholarships and by engaging members of academic institutes as consultants. We are optimistic that the universities will succeed in adapting their teaching agendas to the needs of today and the future in such a way that chemists will be sufficiently prepared to meet their challenges and to fill the positions needed by the chemical industry in the future.

Conference Report

International Conference on Green Chemistry: Challenging Perspectives

The *Green Chemistry: Challenging Perspectives* Conference was sponsored by IUPAC and co-sponsored by the American Chemical Society (ACS), the US Environmental Protection Agency (EPA), the United Nations Educational, Scientific and Cultural Organization (UNESCO), and with support from the European Commission, Directorate General XII—Science, Research and Development: Directorate D-RTD Actions: Environment.

The Conference was organized by Prof. Pietro Tundo and his colleagues from the University of Venice, Italy, during Sunday 28 September to Wednesday 1 October 1997.

Venice is a fascinating city between sea and sky and can be likened to Venus rising from the waves. It is a truly international tourist city drawing visitors by her charm of water and pellucid light. It is free of dust as there are no terrestrial motor vehicles—all transport is by her many canals. However, there are obvious signs of air pollution from the many motor boats, and severe indications of water pollution, corrosion and especially erosion of many of the fine buildings.

Venice offers unrivalled intellectual pleasures derived from masterpieces which mark the meeting of East and West. The varnished greatness of Venice accounts for the myth of an artificial, voluptuous and, perhaps, a tragic city, the sense of intrigues plotted in an atmosphere of corruption where dreams have become nightmares—this is how it can be described by romantics.

Whilst Venice invites *farniente* (idleness) and strolling, this was not the case at this Conference. Prof. Tundo and his team had met the challenge of following the 1997 *Green Chemistry and Engineering Conference*, held in Washington, DC, with the objectives of addressing and finalizing innovative public and private research programmes towards the development of new clean chemical processes.

UNIVERSITÀ CA' FOSCARI DI VENEZIA

Topics

This four-day event covered general, social and technical sessions and covered the following topics:

Chemical Processes: State of the Art for the Environment. Topics included recent developments in environmentally friendly resources and some recent industrial applications.

Inherently Safe Processes. This was related to research performed within the objective of reducing the risks associated with chemical processes and the objective of obtaining profitable, or at the very least, cost-neutral sustainable development.

Inherently Safe Products. The design of safer chemicals is both straightforward and complex. This session addressed the problem of the reduction in the toxicity (and ecotoxicity) of known chemicals without sacrificing efficiency, and the problems associated with the design and invention of new and intrinsically safe molecules.

Catalysis and Biocatalysis. This session discussed new procedures to create alternative synthetic and biosynthetic pathways which can substitute existing processes, which utilize renewable sources, and which operate under mild conditions and at lower costs.

Solventless Processes and Alternative Solvents. This session considered: alternative reaction conditions which have a significant effect on pathways involving overall environmental impact; use of supercritical fluids; and reactions promoted by new irradiation methods.

Chemical Research Policies. Dr Paul Anastas (US-EPA) led this session by introducing different aspects of the policies that govern academic and industrial environmentally compatible chemical research. Particular stress was given to the European Commission and the CEFIC Green Thematic networks in comparison with how similar policies are being developed in the US.

Opening Ceremony

The Opening Ceremony was held at the magnificent Auditorium of the San Margherita on the evening of Sunday 28 September 1997.

Prof. Tundo, in his initial remarks, stressed the immense global and growing significance of 'Green Chemistry', especially for the chemical and all related industries.

Dr Paul Anastas emphasized the initiatives in the

USA, especially the 'President's Green Chemistry Challenge, Awards and Grants for Industry', in particular improvements to the natural environment.

Dr Joseph J. Breen, Executive Director of The Green Chemistry Institute, developed these themes, including the massive support being given by the American Chemical Society.

Prof. Gianfranco Scorrano gave the welcoming address on behalf of IUPAC and indicated the means by which IUPAC was emphasizing its environmental chemistry activities, especially through the Company Associate Scheme and the Chemistry and Environment Division.

The evening's activities concluded with a buffet and a musical concert.

Conference Introduction

The Conference itself was held in the equally and very tranquil surroundings of the Ca'Dolfin Palace of the Universita Ca'Foscari' di Venezia, Calle Della Saoneria.

Prof. Tundo stressed that the ultimate goal of 'Green Chemistry' research is to develop and institute alternative syntheses for important industrial chemicals. This entails the challenge of designing new syntheses and extraction procedures that are less polluting.

It is of the greatest importance to collect all the available data on chemical processes of industrial importance, bearing in mind that older processes are the 'backbone' of facilities available in developing/industrializing and especially the least developed countries. These countries need to heed the experiences of the highly developed countries and thus 'leap-frog' to the newer, cleaner, more economic and less polluting production methods. The chemical industry needs to anticipate the evolution of international regulations and needs to overcome this by a new approach to pollution prevention.

A working party for Environmental Organic Chemistry within IUPAC Commission III.2 on Physical Organic Chemistry under the Chairmanship of Prof. Tundo has included a project on 'Reaction Pathways and Processes in Green Chemistry'. This project is being undertaken in collaboration with the IUPAC Chemistry and Environment Division. It is extremely timely, as every chemical company has its own programme for achieving environmental requirements. However, the dissemination of information in this field can accelerate the process by stimulating competition.

To achieve this goal it is proposed to collect data on the cooperation of the international agencies (e.g. the UN agencies, the EC), industry (chemical, agrochemical, pharmaceutical, etc.), national agencies (e.g. CEFIC and the EPA), in addition to the national chemical societies. It will be essential that each step taken will result in the creation of a policy for sustainable development, by listing the objectives, e.g. elimination of chlorine derivatives, replacement of organic solvents, oxidation reactions, recycling, atom economy, catalysis, biocatalysis, etc.

Opening Address

This was given by Prof. Maurizio Rispoli, President of the University of Venice.

He emphasized that recent years had witnessed the birth of awareness towards the development of industry, of products and of production processes, especially in view of the needs of sustainability.

He stressed the need for attention to be given to the problem of maintaining a dynamic balance between economic development and with due respect for the environment.

It is well known that the chemical industry, including in particular the petrochemical industry, has become the driving force of economic development over the past 100 years; by providing new materials and products which, due to their accessible prices, can satisfy a wide market demand. This development has allowed for improvement in living conditions for consumers.

However, over the past few years, we have begun to question ourselves on the consequences of the devel-

opment, especially certain production processes, which are empirically and theoretically suspected of causing damage to the ecosystem and to the health of people, animals, plants and all organisms on which mankind depends.

Due to this new sensibility towards the value of life, the chemical industry has found itself in the state of needing to comply with health and environmental regulations. However, now is the time for industry to look at 'Green Chemistry', and view the many challenges as *opportunities*, for new investments, new processes and products; but never view these activities as *impediments*.

The chemical companies that will be able to promote and develop these kinds of approach will be the ones that will gain solid competitive advantages.

Simultaneously, researchers can and must find in this environmental challenge, and in the challenge of 'Green Chemistry', a rewarding field of significant opportunities, where the first to succeed will have a very clear advantage.

Conference Résumé

The Conference was attended by 140 delegates from 12 countries. The working sessions were developed to a series of plenary, invited, technical sessions and lectures. There was also a poster session.

The plenary lecture titles were: Bart Drinkenburg (The Netherlands)—*Green Engineering: Opportunities and Realism*; Ugo Romano (Italy)—*Process and Product Innovations for the Development of Environmentally Compatible Technologies*; Terrence J. Collins (USA)—*The Design of Green Oxidants*; Bernard Witholt (Switzerland)—*Organic Chemistry via Biocatalysis*; Joseph M. De Simone (USA)—*Design and Application of Surfactants for Carbon Dioxide: From Polymer Synthesis to Cleaning/Extractions.*

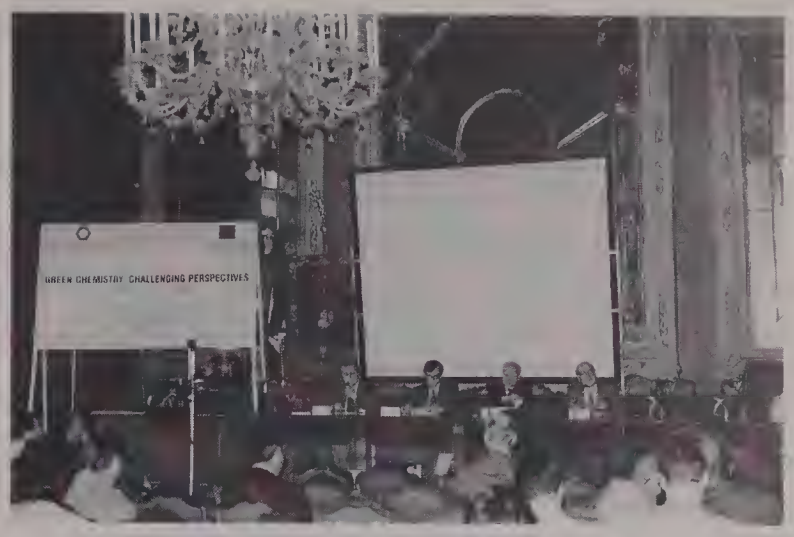
They were supported by 17 oral, nine invited, seven technical session lectures and 24 posters.

With the support of the Italian Enterprise 'Enirerche', Prof. Tundo had published extended summaries of all of the contributions. It is planned for Conference proceedings to be published by the Oxford Science Publications in Spring 1999.

Inter-university Consortium—Chemistry for the Environment

On Monday 29 September 1997 the Conference participants were invited to join the official inauguration of the recently completed laboratories of the Inter-university Consortium, *Chemistry for the Environment*, located in the Science and Technology Gateway in Marghera.

It took place in the presence of senior representatives



of the Italian Government, including Paolo Costa (Secretary of Public Works), Giovanni Castellani (President of the Parliamentary Cultural Commission) and Giuseppe Tognon [Under-secretary of Ministerero dell' Universita e della Ricerca Scienfica (MURST)], who are interested in promoting the development of environmentally friendly technologies, particularly in the highly endangered area surrounding Venice.

Conference Conclusions

In summarizing the Conference Prof. Tundo emphasized:

- The work to be undertaken by the IUPAC Working Party on 'Reaction Pathways and Processes in Green Chemistry'
- The need for industry to adopt the use of new organic (green) processes
- International cooperation

The latter would involve liaison with the international agencies, especially the United Nations Industrial Development Organization (UNIDO) and the United Nations Educational, Scientific and Cultural Organization (UNESCO), and the IUPAC Joint Training Program for Safety and Environmental Protection in Chemical, Pharmaceutical and Bio-Technological Research and Production.

Future collaboration would also be maintained between Prof. Tundo, the new University Consortium, the EPA and EC-DGXII.

Prof. Tundo would also open a newsletter via his E-mail: inca@unive.it, URL web site: http://www.unive.it/inca.html

Initial plans are to be considered for a second conference on 'Green Chemistry' in 1999.

Mervyn Richardson
Birch Assessment Services for Information on Chemicals (BASIC)—Tel./Fax: +44 (0) 1923 774187

Air Pollution Profile of Turkey

As is the case with all environmental problems, the two primary causes of air pollution in Turkey are urbanization—which has been rapid since the 1950s—and industrialization. Before industrialization more than 80% of the population lived in rural areas; now more than 60% live in the cities and industrial complexes. Among the developments contributing to air pollution in the cities are incorrect urbanization for the topographical and meteorological conditions, incorrect division of urban land into lots, low quality fuel and improper combustion techniques, a shortage of green areas, an increase in the number of motor vehicles and inadequate disposal of wastes.

An environment law was brought into effect in 1983. Air pollution standards are determined by the Prime Ministry Environment General Directorate; the pertinent regulation was brought into effect on 2 November 1986. Emission limit values relate mainly to SO_2, CO, NO_2, NO, O_3, total suspended particulates (TSP), hydrocarbons, lead, cadmium and thallium.

Combustion of coal and various kinds of heating oil cause excessive air pollution in Istanbul, Ankara, Bursa and Erzurum during the winter months. Cities in Turkey with significant levels of SO_2 and TSP in the winter months of 1990–94 are shown in Figs 1 and 2.

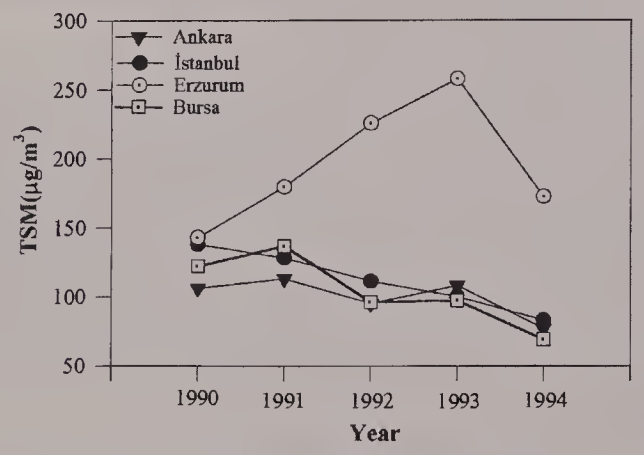


Fig. 1 Average concentration of total suspended matter in 1990–94 winter months in some cities (μg/m³)

Although attention has been given in recent years to the problem of air pollution created by industrial installations, only 6.3% of existing plants have installed necessary equipment to prevent environmental pollution.

Industrial sources of air pollution in Turkey are mainly the fertilizer, iron and steel, paper and cellulose, sugar, cement, textile, petrochemical, pesticide, leather and energy production industries. Average yearly levels of SO_2 and total suspended matter emitted by the main polluting industries are given in Table 1.

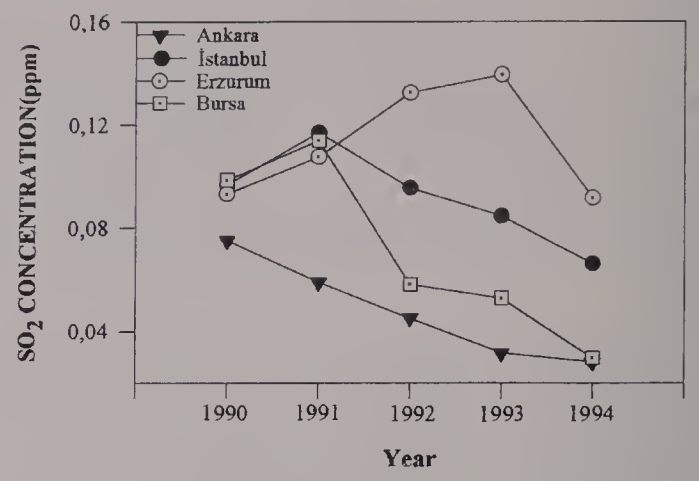


Fig. 2 Average concentration of SO_2 in 1990–94 winter months in some cities (ppm)

Concentrations of O_3, NO_x, SO_x and particulate matter were measured in the Uludag National Park, well known as a ski resort and the highest mountain of west Turkey. The aims of these measurements were to track the transportation of the main air pollutants from Europe to Turkey and to investigate the influence of acid rain on the forest of the Uludag National Park (a Eurotac project).

Table 1 Average yearly levels of SO_2 and particulate matter emitted from the main polluting industries (ton/year)

Industry	Particulate matter	SO_2
Power plants	3940 000	1430 000
Iron & Steel	3330 000	–
Cement	2270 000	32 000
Sugar	290 000	49 000
Metal	5200	30 000
Fertilizer	14 000	30 000

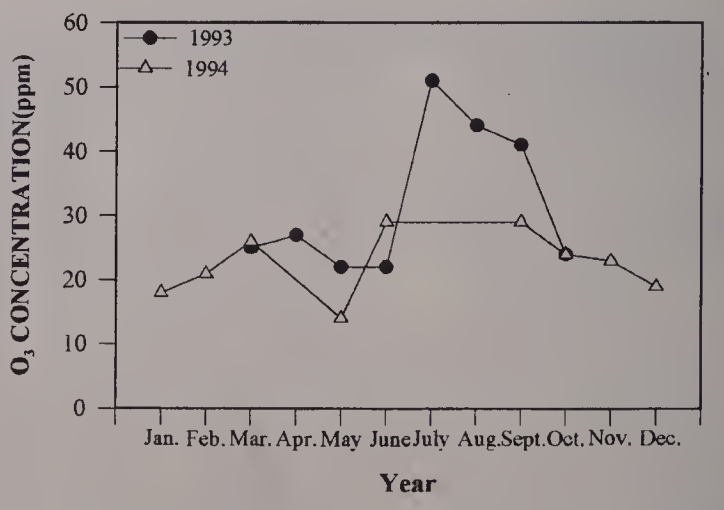


Fig. 3 The concentration of O_3 between 1993–94 which is measured in Uludag National Park (ppm)

An air pollution monitoring station was set up in the Sarialan region (40°10′N 20°08′E) of the Uludag National Park. Ozone concentrations were measured under various meteorological conditions for two years from March 1993 to 1995. During the summer months, the ozone concentrations were rather high due to the transport of photochemically produced ozone precursor gases from the urban and industrial areas. Ozone peaks observed during the night were due to stratospheric injection. Figure 3 shows the concentrations of ozone measured in the Uludag National Park between 1993 and 1994.

References

1 Environmental Profile of Turkey. *Air Pollution*. Environmental Problems Foundation of Turkey Publication, 1995, pp. 39–89.

2 Semra G. Tuncel, A. Hadi Baykal, Gürdal Tuncel and Ulviye Özer. Measurement of NO_x, SO_2, SPM and O_3 at a high altitude station in Northwestern Turkey. *Israel Journal of Chemistry*, 1994, **34**, 403–409.

Ulviye Özer, Rahmiye Aydin and Hasan Akçay
Department of Chemistry, Uludag University, Bursa, Turkey

News

Relocation of IUPAC archival material

In the previous issue of *Chemistry International* (September 1997, pp. 161–163), details were given of the transfer to the Chemical Heritage Foundation (CHF) in late 1996 of much of the IUPAC archival material collected at Oxford over the past nearly 30 years.

In September 1997, E.W. (Ted) Godly, Secretary (1989–93) of the Commission on Nomenclature of Organic Chemistry (CNOC), visited the IUPAC Secretariat at Oxford and deposited a set of minutes for meetings of CNOC during 1966–95, CNOC Secretarial correspondence during 1990–96, nomenclature queries during 1989–95, and draft recommendations for *Revised Nomenclature for Radicals, Ions, Radical Ions and Related Species*; *Glossary of Class Names of Organic Compounds and Reactive Intermediates Based on Structure*; and the *Guide to IUPAC Nomenclature of Organic Compounds*. This carefully consolidated material was passed to CHF with the final archival material from Oxford at the end of October (full details to be included in a future issue of *Chemistry International*).

E.W. (Ted) Godly

Retiring Officers of IUPAC Division Committees and Commissions and of Standing Committees are urged to send similar consolidated material to Elizabeth Swan, Director of Library Services, at the Chemical Heritage Foundation, 315 Chestnut Street, Philadelphia, PA 19106-2702, USA. Tel.: +1 (215) 925 2222 ext 226. E-mail: eswan@chemheritage.org.

'White Book' on endocrine disrupters

In recent years, the hypothesis has been raised that certain chemicals in the environment originating from agricultural, domestic, industrial and natural resources might adversely affect the health of human and wildlife populations by interfering with endocrine (hormonal) systems.

Most of the evidence comes from studies with laboratory animals and observations on wild species. Evidence for effects in humans is far more controversial, or unconvincing, although some scientists have alleged that the public health may be harmed by exposure to low levels of a multitude of chemicals which mimic the function of female sex hormones called oestrogens. More research is needed to answer many questions raised by this hypothesis. However, there is yet no proof that any environmental oestrogen is impacting public health.

As IUPAC has contributed to the debate on the effect of chlorine and chlorine-containing compounds on the environment by publication of Volume 68, No 9, of *Pure and Applied Chemistry*, September 1996, we have begun preparation of an independent and unbiased publication on the 'Endocrine Disrupter' issue. Drawing upon scientific experts from around the world, and in cooperation with IUPHAR and IUTOX, we hope again to put into scientific perspective an issue which has important environmental, societal, economic and industrial implications.

Dr J. Miyamoto

As with the chlorine debate, the Union wishes to encourage the development of a sound scientific base on this immensely complicated issue, urges the public authorities to make relevant decisions on the basis of sound science and not on emotional reactions, and urges industry to act responsibly, endorsing product stewardship and responsible care.

A.E. Fischli, President
R.P. Martin, Committee on Chemistry and Industry Chairman
J. Miyamoto, Chemistry and Environment Division, President

New Executive Director of ICSU

Jean François Stuyck-Taillandier has been appointed Executive Director of the International Council of Scientific Unions (ICSU) for an initial two-year period. A French national with a thorough knowledge of English, Jean François comes from the Collège de France (the French Academy Complex) in Paris, where he was in charge of international relations. Previously he was Science Counsellor at the French Embassy in Tokyo and before that, Director for International Relations of the French National Research Centre (CNRS).

Jean François has a background in physics and chemistry, and has devoted most of his career to international scientific affairs, through which he has acquired familiarity with ICSU and with many of ICSU's members and organizations.

International Newsletter on Chemical Education

Issue No 45 (1997) of the International Newsletter on Chemical Education (INCE) focuses on small-scale chemistry and particularly on affordable experimentation in chemistry. Included are five articles on the topic: *Some thoughts on practical work in chemistry* and *Getting started in small-scale*, by Stuart W. Bennett of the Open University, Milton Keynes, UK; *Innovative tools in small-scale chemistry* by S. Bhanumati of Delhi University, India; *Dedicated glass apparatus* by Stephen Breuer of the University of Lancaster, UK; and *Radmaste microchemistry kits: hands-on practical work for all* by Prof. John Bradley and colleagues from the Radmaste Centre at the University of Witwatersrand, Johannesburg.

This is the first issue produced under the new joint editorship collaboration between Dr Stuart Bennett and Prof. John D. Bradley. The new editors' opening remarks pay tribute to Peter Towse of the University of Leeds, UK, who stepped down after 10 years in the Editor's chair with publication of Issue No. 44. The new editors also take the opportunity to request ideas and articles to shape future issues. Not all issues will have a single theme like No. 45, they say, but seek views on the suggestion that it may be appropriate for every other issue to have a common theme.

Jean François Stuyck-Taillandier

For further information, suggestions or opinions, please contact: Dr Stuart W. Bennett, Department of Chemistry, Open University, Milton Keynes MK7 6AA, UK. Fax: +44 (0) 1908 653744. E-mail: s.w.bennett@open.ac.uk, or Prof. John D. Bradley, Radmaste Centre, University of Witwatersrand, Private Bag 3, Wits 2050, Johannesburg, South Africa. Fax: +27 11 339 7967/1054. E-mail: bradley@aurum.chem.wits.ac.za

IUPAC colleagues deceased

Canada: Dr G. Waddington (18 March 1996), President of Physical Chemistry Division (1969–73), Physical Chemistry Division Committee (1963–69), Committee on Statutes and Bylaws (1972–75), Commission on Physicochemical Symbols, Terminology, and Units (1967–71), Commission on Thermodynamics (1957–69).

South Africa: Prof. M.M. Zulu (18 October 1997), Commission on Nomenclature of Inorganic Chemistry (1989–).

Commission News

Summary Minutes from the Meeting of the Commission on Chemical Kinetics (I.4), Geneva, Switzerland, 24–25 August 1997

Major data evaluation projects of importance in environmental chemistry have been extended and new projects initiated in related areas of environmental science. One, concerned with the thermodynamics of free radicals, was proposed in support of the ongoing projects on atmospheric and combustion data evaluation. Others involve chemistry under extreme conditions and catalysis.

The Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry has continued with its series of evaluations. The most recent supplement (number V) was completed in early 1995, but published only in early 1997 (*J. Phys. Chem. Ref. Data* 1997, **26**, 509–1011) due to problems in the journal production process. Supplement VI has been submitted for publication and should appear this year. Supplement VII is expected to be submitted to the journal by the end of this year. The most recent publication is the sixth major data evaluation published in this series, which is extensively used in mathematical models of the stratosphere and troposphere.

The Subcommittee on Aqueous Solution Kinetics Data for Atmospheric Chemistry has assembled an international panel of experts to evaluate data relevant to atmospheric chemistry taking place in the aqueous phase. The project Evaluated Chemical Kinetic Data for Combustion Chemistry has assembled a working party, tasks have been assigned, and a publication planned. The project Task Force on the Thermodynamics and Chemical Data Base for Hazardous Waste Processing will complete its work this year and a report will be issued in early 1998.

The next meeting will be held in Berlin, Germany, in August 1999.

Dr John T. Herron
(Chairman, Commission I.4)

Summary Minutes from the Meeting of the Subcommittee on Transport Properties, Boulder, Colorado, USA, 21–22 June 1997

Nine scientific presentations were made on specific topics related to the ongoing projects of the Subcommittee.

Standard Reference Data for the Transport Properties of Fluids. New recommendations for the viscosity and thermal conductivity of methane were concluded. The resulting paper, reviewed by two members of the Subcommittee, will be published under the Subcommittee auspices.

Work that will continue refers to propositions for recommendations for the:

a viscosity of liquid water
b viscosity of toluene
c viscosity and thermal conductivity of methane + ethane
d viscosity and thermal conductivity of butane
e viscosity of steam
f viscosity of *n*-pentane

Standard Reference Value for the Viscosity of Water. A new proposition from ISO for a new value for the viscosity of water was considered and not agreed. A detailed case underlying the reasons for the disagreement was prepared for ISO.

Midas Databank of Transport Property Data. It is hoped that the work carried out by Prof. K. Stephan and R. Krauss in compiling all recent and unpublished results on transport property measurements will be continued normally.

Round Robin Project on R134a. The project aiming to reconcile the profound differences of the transport properties of R134a between the data obtained in different countries within IUPAC has been completed. A paper illustrating this point will soon be published under the Subcommittee's auspices. The Subcommittee is grateful for the financial contribution of IUPAC to this project.

Prof. Marc J. Assael
(Secretary, Subcommittee on Transport Properties)

Summary Minutes from the Meeting of the Commission on Biotechnology, Geneva, Switzerland, 23–24 August 1997

During two sessions, one with the Titular Members and Dr Nara, and a second with the additional presence of Dr Chorgade, Prof. Hearn and Dr Kiener, the mission statement and future activities of the recently reconstituted Commission on Biotechnology (COB) were discussed with the following results:

1. The mission of COB

- to enhance the understanding of modern biotechnology among chemists world-wide;
- to foster the integration of biochemistry and biotechnology within IUPAC;
- to serve both industrial and public interests.

2. Projects

There was consensus to concentrate on just a few but highly profiled projects.

COB Home Page. Establish a COB Home Page (linked to the IUPAC Home Page. Contains general information on COB members and projects. Will be placed on the new IUPAC server at the University of Chapel Hill, NC).

Biotechnology browser, web page. Establish a web page which informs chemists world-wide about basic methods, trends and advances of modern biotechnology. Original graphs, in their original language, will be used from: (a) national education series on biotechnology (available from the USA, Japan, Germany, France, the UK, Switzerland, etc.), and (b) from selected monographs. Financial support will be solicited from the pertinent publishing houses. This web page further contains addresses of national organizations providing information material on modern biotechnology.

National patent regulations in biotechnology, web page. Establish a web page which provides information about national/regional regulations on patenting in biotechnology on a world-wide basis. The project addresses individual inventors, start-up companies and medium and small enterprises and is strictly limited to information; no attempts will be made to harmonize existing patent rules. The web page contains the addresses of biotechnology-related branches within the national patent offices (if available) and the addresses of national patent law firms specializing in biotechnology-related patent applications. Financial support of the latter group will be solicited.

Nomenclature rules for recombinant proteins, jointly with IUBMB. Develop nomenclature for isoforms, glycoforms, genome-derived proteins, artificial proteins obtained by gene shuffling, etc., with a particular view on patent issues.

Organize two sections or satellite meetings at the IUPAC Biotechnology Conference in Berlin 2000. The project is aimed at improving the interface among chemists and biologists. Two topics will be chosen which are relevant to either professional group but lack mutual penetration, such as 'Prediction of properties of genome-derived proteins by the use of bioinformatics, e.g. surface/charge modelling' and 'Proteomics in drug development'.

White Book or Monograph on 'Metabolic engineering and the production of chemicals'. The feasibility to produce bulk and speciality chemicals (e.g. solvents, vitamins, dyes, intermediates) through modern biotechnology at competitive economics by applying metabolic flux analysis and genetic engineering will be analyzed in view of national and regional differences in raw material prices, competitive processes, access to technology, etc.

PAC article. A chemical product will be chosen which can either be produced by organic synthesis or biotransformation/fermentation, and the ecobalances of both processes will be compared.

3. Other discussion points

3.1. IUPAC Biotechnology Conference 2004

According to IUPAC traditions, the meeting should be held in the American hemisphere. Following a letter of the former chairman of COB to the pertinent national IUPAC organizations, interest to act as a host to this conference has been expressed by Chile and Canada. While a majority of the present COB members showed a tendency to favour Chile, the available information is too scarce to allow for any decision yet. COB Chairman will (a) collect more information, (b) contact the putative organizers in Chile and Canada on the basis of an IUPAC questionnaire and the regional potential to attract scientists with high profile.

3.2. Functions and membership

The participants agreed to propose to Dr Michelle Browner the position of COB's Vice-chairperson.

COB Chairman requests IUPAC Secretariat to assign Dr Nara as a Titular Member of COB.

The membership of COB should not exceed 15 persons, and about half of the members should work in industry. COB chairman will initiate contacts to individuals with the desired profile and nationality, followed by their nomination as national representatives through their national adhering organizations.

Prof. Rolf Schmid
(Chairman)

Summary Minutes from the Meeting of the Commission on Soil and Water Chemistry (VI.3), Geneva, Switzerland, 23–25 August 1997

The major topics extensively discussed during this meeting were the composition of the Commission and the progress of the current projects. The main activity to be carried out by the Commission in the near future will be the organization of a conference on 'Degradation Processes in the Environment' to be held in Dubrovnik, Croatia, May 1998.

Since the last meeting of the Commission (Schmallenberg, Germany, September 1996), two draft contributions to *Pure and Applied Chemistry* were completed, entitled *An overview of analytical quality control and quality management in water laboratories* and *The importance of natural organic material for environmental processes in waters and soils*. Also a report was produced, containing the main findings of the workshop on *The importance of natural organic material for environmental processes in waters and soils*, which was held in Germany in September 1996. Thereupon the scientific findings of the workshop were prepared for publication.

During the meeting in Geneva several ideas for new projects and possibilities for new feasibility studies were discussed. In line with the recommendations from the Chemistry and the Environment Division it was decided to limit the number of projects, in order to warrant their successful completion.

The following areas were identified as being of potential interest to the work of the Commission.

1 Disinfection and disinfection products from water treatment
2 Pesticides appearance in drinking water resources—joint action is needed with the Agrochemicals Commission (VI.2) and Commission VI.1 (to cover analytical aspects)
3 Atmospheric deposition in drinking water reservoirs
4 Antibiotics in the environment and drinking water: effects and occurrence
5 Statistical performance standards of analytical methods for soil and water analysis
6 Chemical properties of sewage sludge

No additional action on the proposed new projects was taken. Commission members are requested to submit additional ideas before March 1998 in order to enable discussion of all proposed new projects during the next meeting.

The next meeting will be held one day before the start of the conference on 'Degradation Processes in the Environment', Dubrovnik, Croatia, 23 May 1998.

Dr W. Peijnenburg
(Secretary)

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most recent list of the national/regional centres appears in *Chemistry International* 1995, **17**, 141.

Extension and revision of the nomenclature for spiro compounds

Spiro ring systems have two or more rings linked by one common atom. Several different methods are used to name such systems. Rules A-41, A-43, B-10 and B-12 (*Nomenclature of Organic Chemistry*, 1979) describe the basics of how to name these compounds. The alternative methods in rules A-42 and B-11 are abandoned.

This document describes the nomenclature in greater detail and extends it to cover branched polyspiro systems and compounds where three rings have one common spiro atom. A new notation, based on the von Baeyer method of naming spiro systems where all components are monocyclic, allows both linear and branched polyspiro systems to be named without ambiguity. It also enables the names to be readily interpreted.

Comments on these recommendations are welcome and should be sent by 31 March 1998 to: Dr G.P. Moss, Department of Chemistry, Queen Mary & Westfield College, Mile End Road, London E1 4NS, UK. Tel.: +44 (0) 171 975 5555 ext 3718. Fax: +44 1081 981 8745 (Chemistry) or +44 (0) 171 975 5500.

Extension and revision of the von Baeyer system for naming polycyclic compounds (including bicyclic compounds)

It has been recognized for some time that the von Baeyer system for naming polycyclic ring systems described in Rules A-31, A-32 and B-14 (*Nomenclature of Organic Chemistry,* 1979) has deficiencies. This document describes how to name any polycyclic ring system by the von Baeyer system. It extends the previous rules and provides guidance on the naming of ring systems which previously the rules did not cover.

The method is to identify the main ring and main bridge which provide the basic bicyclic system and numbers these atoms. Then all further bridges, whether or not they include additional atoms, are identified by indicating not only the number of atoms but also the two atoms to which the bridge is attached. The final name also indicates the total number of rings and the total number of atoms in the ring system. Heteroatoms, unsaturation and substituents are shown in the usual way.

Comments on these recommendations are welcome and should be sent by 31 March 1998 to: Dr G.P. Moss, Department of Chemistry, Queen Mary & Westfield College, Mile End Road, London E1 4NS, UK. Tel.: +44 (0) 171 975 5555 ext 3718. Fax: +44 1081 981 8745 (Chemistry) or +44 (0) 171 975 5500.

Analytical aspects of chemically modified electrodes: classification, critical evaluation and recommendations

Chemically modified electrodes (CMEs) for analytical chemistry applications are classified and evaluated. Several analytical aspects of CMEs are critically reviewed. These include effects, such as analyte and/or reagent accumulation on the electrode to increase selectivity and detectability, and/or chemical transformation of the analyte to a form which is more suitable for its determination, electrocatalysis with the immobilized catalyst or analyte, permeability of neutral and ionic analyte or reagent, ionic equilibria of analyte and/or reagent, controlled analyte or reagent releasing as well as change of the electrode mass. Also, suitable definitions are provided and recommendations formulated for the most effective analytical use of CMEs. In a previous report prepared in the Commission on Electroanalytical Chemistry by R.A. Durst, A.J. Baeumer, R.W. Murray, R.P. Buck and C.P. Andrieux (*Pure Appl. Chem.* 1997, **69**, 1317), general terminology, definitions and methods of preparation of CMEs have been described and classified as well as relevant recommendations provided.

Comments on these recommendations are welcome and should be sent by 31 March 1998 to: Dr W. Kutner, Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44, 01-224 Warsaw, Poland. Tel.: +48 22 632 32 21, ext. 3217; Fax: +48 22 632 52 76; E-mail: wkutner@ichf.edu.pl

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry.*

Nomenclature and terminology of fullerenes: a preliminary survey

Synopsis

Some difficult problems are encountered with fullerene molecules, in particular with regard to numbering, the description of isomers having the same symmetry, the question of describing ring systems attached to the fullerene structure, and indeed how to define a fullerene adequately in the first place. A set of proposals is presented for naming the principal fullerene structures and some of their derivatives, using IUPAC nomenclature principles and practices insofar as they can be taken to apply, together with usages developed by the Chemical Abstracts Service (CAS), cited wherever such comparison has been considered useful.

This Report was prepared for publication by E.W. Godly (10 Lawrence Avenue, New Malden, Surrey KT3 5LY, UK) and R. Taylor (Chemistry Laboratory, CPES Building, University of Sussex, Falmer, Brighton BN1 9QJ, UK). *The full details are to be found in* Pure Appl. Chem. *1997, **69**, 1411–1434.*

Nomenclature, symbols, units and their usage in spectrochemical analysis—XVI. Laser-based molecular spectroscopy for chemical analysis—luminescence (IUPAC Recommendations 1997)

Synopsis

This report is the 16th in a series on spectrochemical methods of analysis issued by IUPAC Commission V.4. It is concerned with the use of lasers in molecular spectroscopy dealing with luminescence.

This Report was prepared for publication by T. Vo-Dinh (Health Sciences Research Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6101, USA), N.H. Velthorst (Department of Analytical Chemistry, Free University, 1081 HV Amsterdam, the Netherlands), D.S. Moore (Chemical and Laser Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA) and B. Schrader (Institut für Physikalische und Theoretische Chemie, Universität-GH-Essen, D-45117, Essen, Germany) for the Commission on Spectrochemical and Other Optical Procedures for Analysis of the Analytical Chemistry Division. *The full details are to be found in* Pure Appl. Chem. *1997, **69**, 1435–1449.*

Nomenclature symbols, units and their usage in spectrochemical analysis—XVIII. Laser-based molecular spectroscopy for chemical analysis: Raman scattering processes (IUPAC Recommendations 1997)

Synopsis

This report is 18th in a series on spectrochemical methods of analysis issued by IUPAC Commission V.4. It is concerned with Raman scattering processes, usually induced by lasers, covering the UV, visible, and near infrared spectral regions. Raman scattering can be divided into linear and non linear processes. Due to their importance for chemical analysis, mainly the linear Raman effects are treated.

This Report was prepared for publication by B. Schrader (Institut für Physikalische und Theoretische Chemie, Universität-GH-Essen, D-45117 Essen, Germany) and D.S. Moore (Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA) for the Commission on Spectrochemical and Other Optical Procedures for Analysis of the Analytical Chemistry Division. *The full details are to be found in* Pure Appl. Chem. *1997, **69**, 1451–1468.*

Analytical chiral separation methods (IUPAC Recommendations 1997)

Synopsis

In recent years there has been considerable interest in the synthesis and separation of enantiomers of organic compounds especially because of their importance in the biochemistry and pharmaceutical industry. Frequently the methods used for the separations, for monitoring the progress of an asymmetric synthesis or optical purity of the products are chromatographic with liquids, gases or supercritical fluids as the mobile phase. More recently capillary electrophoresis has

been added as an analytical chiral separation method. These applications have led to a number of terms and expressions in addition to those commonly used or recently recommended for the chemistry and physical properties of chiral compounds. This Nomenclature provides the descriptions and definitions for additional terms particularly related to analytical separation methods, and to the formation and enantiomeric purity of chiral products.

This Report was prepared for publication by Vadim A. Davankov (Nesmeyanov-Institute of Organo-Element Compounds, Russian Academy of Sciences, Moscow 117813, Russia) for the Commission on Separation Methods in Analytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1469–1474.*

Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology (IUPAC Recommendations 1997)

Synopsis

A wide range of stationary phases and column packing materials have been developed over the years for liquid chromatography and these need to be described accurately and unambiguously. The present paper, which is the first of a series planned for this area, recommends terms for the description of the stationary phase materials and their properties and expands the list of terms given in Nomenclature of Chromatography (*Pure Appl. Chem.* 1993, **65**, 819–872). It concentrates on the chemical properties and chromatographic role of the materials. Many of the terms to describe their physical properties as particles have been discussed in a recent paper on the characterization of porous solids (*Pure Appl. Chem.* 1994, **66**, 1739–1758).

This Report was prepared for publication by Roger M. Smith (Department of Chemistry, Loughborough University, Loughborough, Leics. LE11 3TU, UK) and Aurél Marton (Department of Analytical Chemistry, University of Veszprém, PO Box 158, H-8201, Veszprém, Hungary) for the Commission on Separation Methods in Analytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1475–1480.*

Classification and characterization of stationary phases for liquid chromatography: Part II. Characterization of ion exchange chromatographic stationary phases (IUPAC Recommendations 1997)

Synopsis

In order to characterize ion exchange chromatographic stationary phases, the thermodynamic exchange constant and the free energy interaction parameters are recommended. These parameters are calculated from the experimentally available corrected selectivity coefficient vs. exchanger phase composition functions. The equations used for the calculations have been obtained by introducing the Friedman equation (developed for the calculation of the excess free energy change) into the thermodynamic derivation. The suggested parameters also make possible the estimation of the value of the selectivity coefficient at an arbitrary exchanger phase composition. The characteristic parameters of the ion exchange resins and the equations in a directly suitable form for the estimation of the selectivity coefficient are calculated and presented for several systems.

This Report was prepared for publication by Aurél Marton (Department of Analytical Chemistry, University of Veszprém, PO Box 158, H-8201, Veszprém, Hungary) for the Commission on Separation Methods in Analytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1481–1487.*

Critical survey of stability constants of complexes of thiocyanate ion (Technical Report)

Synopsis

Presented is a review of the stability constants for metal complexes with thiocyanate ion. The literature data presented are critically discussed and recommended values, where warranted, listed from the many studies cited.

This Report was prepared for publication by Abraha Bahta (Department of Chemistry & Biochemistry, University of California-Los Angeles, Los Angeles, CA 90024-1569, USA), Gordon A. Parker (Department of Natural Sciences, University of Michigan-Dearborn, Dearborn, MI 48128-1491, USA) and Dennis G. Tuck (Department of Chemistry & Biochemistry, University of Windsor, Windsor, Ontario, Canada) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1489–1548.*

Critical survey of stability constants of metal-imidazole and metal-histamine systems (Technical Report)

Synopsis

Thermodynamic data for the proton and metal ion complexation equilibria of imidazole (1,3-diazole, glyoxaline) and histamine (4-imidoazolethylamine, 4-(2′-aminoethyl)imidazole) have been collected and critically evaluated. The literature search has been performed by using IUPAC's 'Stability Constants Database' and covers the literature until 1992. Important criteria for acceptance comprise specification of the essential reaction conditions, the correctness of calibration techniques and appropriate equilibrium analysis of experimental data. Recommended values with respect to proton–ligand and metal ion–ligand equilibria have been tabulated. Furthermore, the medium dependence of these reactions has been evaluated using an extended Debye–Hückel expression.

This Report was prepared for publication by Staffan Sjöberg (Department of Inorganic Chemistry, Umeå University, S-90187 Umeå, Sweden) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1549–1570.*

The importance of natural organic material for environmental processes in waters and soils (Technical Report)

Synopsis

The role and function of natural organic material (NOM) for the terrestrial and aquatic environment is strongly related to nutrient availability for plants, relevant for crop production, as well as to be a source of energy for macro- and microorganisms, to influence physicochemical conditions of soil and sediments and to buffering and exchange capacity, relevant for the immobilization and mobilization of environmental pollutants. This article reviews the available information about the importance of natural organic material for environmental processes in water and soil. After explaining general terms regarding natural organic material and its chemical structure and presenting the actual state of analytical methods, interactions between environmental variables and the natural organic material as regards its formation and behaviour, as well as interactions between natural organic material and the fate of pollutants in the terrestrial and aquatic environment are discussed emphasizing some relevant processes such as sorption, mobility and bioavailability. Finally some aspects on modelling such processes are presented.

This Report was prepared for publication by W. Kördel (Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, Auf dem Aberg 1, Grafschaft, D-57392 Schmallenberg, Germany), M. Dassenakis (Department of Chemistry, Section III, University of Athens, 15 Athens, Greece), J. Lintelmann (Institut für Ökologische Chemie, GSF Forschungszentrum für Umwelt und Gesundheit GmbH, Postfach 1129, 85758 Oberschleissheim, Germany) and S. Padberg (Fraunhofer-Institut für Umweltchemie und Ökotoxikologie, Auf dem Aberg 1, Grafschaft, D-57392 Schmallenberg, Germany) for the Commission on Soil and Water Chemistry of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1571–1600.*

Calculation and application of coverage intervals for biological reference values: a supplement to the approved IFCC recommendation (1987) on the theory of reference values (Technical Report)

Synopsis

The costs of sampling and analysis of samples are sometimes too high to obtain 120 or more reference values as recommended by the International Federation of Clinical Chemistry (IFCC). Here coverage intervals should be used to give a statistically well defined measure of the uncertainty of the interval. Additionally, when many reference values are available, the coverage interval may provide useful information on the distribution. Hence, extending the IFCC recommendation, the calculation and presentation of the 0.95 coverage interval is recommended, together with information on its coverage uncertainty with a probability of at least 0.95. Non-parametric coverage intervals can be calculated regardless of the distribution of reference values, and parametric coverage intervals can be calculated if transformation of the distribution of reference values to a normal distribution is feasible. The Report gives guidance in calculating both types of intervals. However, in agreement with IFCC, the non-parametric intervals are recommended, thus avoiding the transformation step. A numerical example concerning coverage intervals for blood lead concentration is presented.

This Report was prepared for publication by O.M. Poulsen, E. Holst and J.M. Christensen (National Institute of Occupational Health, Denmark, Lersoe Parkallé 105, DK-2100 Copenhagen, Denmark) for the Commission on Toxicology of the Clinical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1601–1611.*

Biotransformations of non-natural compounds: state of the art and future development

Synopsis

The transformation of non-natural compounds by enzymes—generally referred to as 'biocatalysis'—has evolved as a trend-section of organic synthesis during the mid-1980s. As a consequence, a remarkable number of reliable biochemical techniques have been developed during the last decade, which constitute powerful tools for modern organic synthesis. In this report, the state of the art of biotransformations as well as future developments are critically reviewed with respect to strengths and weaknesses of the existing methods.

This Report was prepared for publication by Kurt Faber (Institute of Organic Chemistry, Graz University of Technology, Stremayrgasse 16, A-8010 Graz, Austria) for the Commission on Biotechnology. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1613–1632.*

Notations and conventions in molecular spectroscopy: Part 1. General spectroscopic notation (IUPAC Recommendations 1997)

Synopsis

The field of molecular spectroscopy was surveyed in order to determine a set of conventions and symbols which are in common use in the spectroscopic literature. This document, which is Part 1 in a series, establishes the notations and conventions used for general spectroscopic notations and deals with quantum mechanics, quantum numbers (vibrational states, angular momentum and energy levels), spectroscopic transitions and miscellaneous notations (e.g. spectroscopic terms).

This Report was prepared for publication by C.J.H. Schutte (University of South Africa, PO Box 392, Pretoria 0001, South Africa), J.E. Bertie (Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2), P.R. Bunker (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada), J.T. Hougen (Molecular Physics Division, National Institute for Standards and Technology, Gaithersburg, Maryland 20899, USA), I.M. Mills (Department of Chemistry, University of Reading, Whiteknights, Reading RG6 2AD, UK), J.K.G. Watson (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada) and B.P. Winnewisser (Justus Liebig Universität, Physikalisch-Chemisches Institut, Heinrich-Buff-Ring 58, D-6300 Giessen, Germany) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1633–1639.*

Notations and conventions in molecular spectroscopy: Part 2. Symmetry notation (IUPAC Recommendations 1997)

Synopsis

The field of molecular spectroscopy was surveyed in order to determine a set of conventions and symbols which are in common use in the spectroscopic literature. This document, which is Part 2 in a series, establishes the notations and conventions used for the description of symmetry in rigid molecules, using the Schoenflies notation. It deals firstly with the symmetry operators of the molecular point groups (also drawing attention to the difference between symmetry operators and elements). The conventions and notations of the molecular point groups are then established, followed by those of the representations of these groups as used in molecular spectroscopy.

This Report was prepared for publication by C.J.H. Schutte (University of South Africa, PO Box 392, Pretoria 0001, South Africa), J.E. Bertie (Department of Chemistry, University of Alberta, Edmonton, Canada T6G 2G2), P.R. Bunker (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada), J.T. Hougen (Molecular Physics Division, National Institute for Standards and Technology, Gaithersburg, Maryland 20899, USA), I.M. Mills (Department of Chemistry, University of Reading, Whiteknights, Reading RG6 2AD, UK), J.K.G. Watson (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada) and B.P. Winnewisser (Justus Liebig Universität, Physikalisch-Chemisches Institut, Heinrich-Buff-Ring 58, D-6300 Giessen, Germany) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1641–1649.*

Notations and conventions in molecular spectroscopy: Part 3. Permutation and permutation–inversion symmetry notation (IUPAC Recommendations 1997)

Synopsis

The field of molecular spectroscopy was surveyed in order to determine a set of conventions and symbols which are in common use in the spectroscopic literature. This document, which is Part 3 in a series, deals with

symmetry notation referring to groups that involve nuclear permutations and the inversion operation.

This Report was prepared for publication by P.R. Bunker (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada), C.J.H. Schutte (University of South Africa, PO Box 392, Pretoria 0001, South Africa), J.T. Hougen (Molecular Physics Division, National Institute for Standards and Technology, Gaithersburg, Maryland 20899, USA), I.M. Mills (Department of Chemistry, University of Reading, Whiteknights, Reading RG6 2AD, UK), J.K.G. Watson (Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa K1A 0R6, Canada) and B.P. Winnewisser (Justus Liebig Universität, Physikalisch-Chemisches Institut, Heinrich-Buff-Ring 58, D-6300 Giessen, Germany) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1651–1657.*

Nomenclature of inorganic chains and ring compounds (IUPAC Recommendations 1997)

Synopsis

A systematic, additive approach to name inorganic chain and cyclic compounds is introduced. The method does not require any prior knowledge about the nature of bonds between the atoms. Though the method can be applied to all compounds, its use is mainly intended for inorganic compounds which are mainly composed of atoms other than carbon. In the case of neutral chain frameworks the compound is called 'catena' preceded by a multiplicative prefix 'di-', 'tri-', etc., to indicate the number of branches in the molecule. Likewise cyclic compounds are called 'cycle' preceded by the appropriate multiplicative prefix. A mixed chain and ring compound is named as 'catenacycle'. In the case of charged species the names are modified by the suffixes '-ium' and '-ate'. The connectivity in the framework is indicated by a nodal descriptor which is placed in square brackets immediately before the terms 'catena', 'cycle' or 'catenacycle'. In simple chain and ring compounds it is permissible to replace the nodal descriptor with a numeric indicator [*n*] when *n* is the number of atoms in the principal chain or ring. The atoms are numbered according to the general nodal nomenclature regardless of their chemical identity. Only in the case of ambiguity is the chemical nature of the atoms taken into consideration. The atoms forming the nodal skeleton are listed in alphabetical order complete with their locants and are named by modifying the element radical names in Table VII of '*Nomenclature of Inorganic Chemistry*' by substituting '-y' for the terminal '-io'. Atoms and groups of atoms which are not a part of the nodal framework are named as ligands and are cited in alphabetical order together with their locants before the cited sequence of the atoms constituting the nodal framework.

This Report was prepared for publication by E.O. Fluck (Gremlin-Institut für Anorganische Chemie und Grenzgebiete der Max-Planck-Gesellschaft, Carl Bosch Haus, Varrentrappstrasse 40–42, D-60486, Frankfurt, Germany) and R.S. Laitinen (Department of Chemistry, University of Oulu, Linnanmaa, FIN-90570 Oulu, Finland) for the Commission on Nomenclature of Inorganic Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1659–1692.*

Characterization of finite length composites: Part I. Introductory paper (Technical Report)

Synopsis

A project representing a sizeable effort of IUPAC Working Party 4.2.1 on two thermoplastic matrices reinforced with three different fibre types and involving two different injection techniques is introduced in terms of its objectives, adopted strategy, materials, main variables, outcome reporting and participating laboratories. The paper outlines details (constituents, composites, injection moulding, mould cavity) common to all undertaken studies. At the same time it summarizes the major outcome in terms of moulding anisotropy and heterogeneity as both controlled by the constituting materials—matrix and fibre and processing conditions used for moulding preparation. More detailed information which is contained in publications dedicated to individual areas under investigation, namely to: (1) mechanical performance of injected moulded composites, (2) studies on thin sections extracted from mouldings (wafers), (3) determination of structural aspects of composites, (4) modelling of stiffness and (5) rheological studies, is referred to in appropriate places.

This Report was prepared for publication by A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) and P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1693–1705.*

Characterization of finite length fibre composites. Part II. Mechanical performance of injection moulded composites (Technical Report)

Synopsis

An overview is given of the mechanical performance (stiffness, strength, toughness, creep...) of finite fibre length reinforced thermoplastics based on polypropylene and polyamide as the matrices and glass, carbon and Kevlar as the reinforcement. Different degrees of fibre orientation distribution and fibre attrition as produced by classical injection moulding and multiple-live feed moulding were evaluated. It was found that the simple test geometry used (injection moulded plaques) resembled more a complicated structure than a material. The properties measured therefore were more the complex response of a strongly anisotropic structure than simple material properties. Increased alignment of the fibres in a given direction affected all the mechanical properties, but the effect was largest for the tensile stiffness. A higher degree of fibre orientation was not accompanied by an increase in properties related to failure (ultimate stress). The modelling of ultimates stress showed that this could be explained by the more severe fibre attrition which resulted from the forces applied to orient the fibres.

This Report was prepared for publication by L. Glas (Shell Research SA, Chemical Research Centre Shell, Louvain-la-Neuve, Belgium), P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK), T Vu-Khanh (Université de Sherbrooke, Faculté des Sciences Appliquées, Département de Génie Mécanique Sherbrooke (Quebec), Canada) and A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1707-1723.*

Characterization of finite length composites: Part III. Studies on thin sections extracted from mouldings (wafers) (Technical Report)

Synopsis

Through-thickness aspects of composites are studied by means of structural investigations and mechanical testing of thin 'wafers' machined from moulded specimens. Two injection moulding regimes, namely the Dynamic and Static mode, have been used to induce different fibre orientations in polypropylene (PP) reinforced with glass (g) and polyamide (PA) reinforced with carbon (c). Novel experimental techniques such as the 'rebound technique', uniaxial compressive yield and flexural testing of circular discs have been used for evaluation of longitudinal and transverse properties. A strong anisotropy of properties in composite mouldings is governed by the spatial fibre orientation. This depends on both the matrix and the processing conditions used with the system PP/g being more regularly structured (skin/core morphology) than PA/c. A satisfactory agreement in the area (a) structure/performance and (b) experiment/theory has been achieved.

This Report was prepared for publication by A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) and P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1725–1740.*

Characterization of finite length composites: Part V. Modelling of stiffness (Technical Report)

Synopsis

This characterization of a range of glass and carbon fibre reinforced polypropylene and polyamide injection mouldings forms part of a wider IUPAC Working Party 4.2.1 study of these materials. In this part of the work we summarize observations of stiffness and microstructural characterization with the aim of linking these features via a micromechanical model. The model makes a number of simplifying assumptions in order to be tractable and is based on calculating the stiffness of a number of 'imaginary' layers through the thickness of the moulding, with each layer having a singular fibre orientation. The stiffness of the moulding is then determined by an appropriate summation of the stiffness of these layers. The agreement between observed and 'modelled' stiffness is reasonable within the context of the assumptions necessary for tractability.

This Report was prepared for publication by P.S. Allan (Brunel University, The Wolfson Centre for Materials Processing, Uxbridge, Middlesex, UK), A. Cervenka (Shell Research BV, Koninklijke/Shell Laboratorium Amsterdam, the Netherlands) and D.R. Moore (ICI plc, Wilton, Middlesbrough, Cleveland, UK) for the Working Party on Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. *1997, **69**, 1741–1751.*

Critical evaluation of the use and analysis of stable isotopes (Technical Report)

Synopsis

The methodology of isotopic analysis is discussed. In the first instance because a choice of analytical methods often conditions the success of research carried out with stable isotopes. The methodology of use is treated in two different chapters according to their resting or not on measurements of isotope effects. In the second case, stable isotopes are specially useful for isotope dilution analysis, studies of transport phenomena, medical diagnoses. Advantages and drawbacks of their use with respect to that of radioactive isotopes are described and examples are given. Usage of isotope effects is a specificity of stable isotope work. Methods of measuring equilibrium and kinetic effects are explained. A discussion is given of tenets of applications in research in pharmacology, geochemical processes, and of kinetic effects in studies of reaction mechanisms, especially in biology. Utilization of nuclear properties, particularly in medicine, are mentioned. This report does not cover techniques of isotope separation, preparation of labelled compounds, uses of isotopes in dating methods or in nuclear industries.

This Report was prepared for publication by Etienne Roth (CEA, SPAM, CE Saclay, 103 rue Brancas, 92310, Sèvres, France) for the Commission on Radiochemistry and Nuclear Techniques of the Analytical Chemical Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1753–1828.*

The determination of trans unsaturated fatty acids in edible oils and fats by capillary gas–liquid chromatography (Technical Report)

Synopsis

Collaborative studies on the application of capillary gas–liquid chromatography for the determination of *trans* unsaturated fatty acids are described. The method investigated involves preparation of methyl esters with methanolic potassium hydroxide followed by analysis of fatty acid methyl esters by gas–liquid chromatography on polar capillary columns. Care has to be taken in selecting working conditions to obtain the best obtainable resolution of signals necessary for reliable identification and determination of *trans* unsaturated fatty acids.

This Report was prepared for publication by A. Dieffenbacher and P. Dysseler for the Commission on Oils, Fats and Derivatives of the Environmental Chemistry Division. The full details are to be found in Pure Appl. Chem. *1997,* ***69****, 1829–1837.*

PAC Review

***Pure and Applied Chemistry* (PAC) is the official journal of IUPAC. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in PAC are published in *Chemistry International* in the section Recent Reports. In this section we take a brief look at symposia and lectures published in recent issues of PAC.**

Lectures from Symposia and Conferences

Carbohydrates

The September 1997 issue of *Pure and Applied Chemistry*, **69**(9), contains texts of the plenary lectures presented at the 18th International Carbohydrate Symposium held in Milan, Italy, 21–26 July 1996. The Symposium was organized by the Organic Chemistry Division in conjunction with the International Carbohydrate Organization, the International Union of Biochemistry and Molecular Biochemistry, the Italian Chemical Society, the Italian Biochemical Society and the Italian Research Council (CNR).

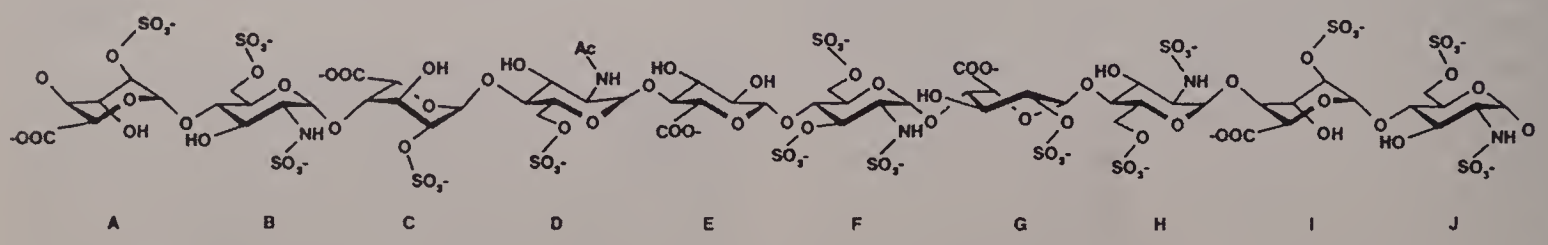
The Whistler Award Lecture was presented by Constant van Boeckel of Organon Scientific Development Group in the Netherlands. His theme was heparin—from the original 'soup' to well-designed heparin mimetics. His lecture traces the history of heparin—from the introduction of heparinotherapy in 1937—to present day. He covers the use of heparin in clinics of the late 1930s, the structure of anti-factor Xa oligosaccharides obtained from heparin, first generation synthetic pentasaccharides and finally second generation synthetic pentasaccharides. He concludes that the chemical synthesis approach has been very fruitful in terms of both understanding the mode of action of heparin and production of potential active substances for new drugs. It is clear, he says, that the interaction of the complex polysaccharide and AT III depends on the presence of a very precise array of sulfate and carboxylate groups that induce a conformational change necessary and sufficient to inhibit blood coagulation factor Xa. More importantly, it is possible to obtain in a pure state all the heparin mimetics desired. These synthetic products constitute active principles for new drugs the biological profile of which can be adapted at will to reproduce some of the many activities of heparin.

The other lectures covered: the emerging importance of oligosaccharide synthesis; the use of low molecular weight carbohydrates as organic raw materials; the information capacity of the carbohydrate code; structural glycobiology; recent progresses in the glycodrug area; shapes and motions of polysaccharide chains; a challenge to the riddle of the carbohydrate chain; heparan sulfate; cell-type specific expression on gangliosides in the central nervous system; and microbial exopolysaccharides.

Physical organic chemistry

The September issue also contains the special and plenary lectures presented at the 13th International Conference on Physical Organic Chemistry held in Inchon, Korea, 26–29 August 1996. The Conference was organized by the Organic Chemistry Division in conjunction with Inha University and the Korean Chemical Society and timed to coincide with the 50th anniversary of the Korean Chemical Society.

The opening paper, a special lecture presented by George Hammond of Bowling Green State University, Ohio, and Georgetown University, Washington DC, provides a historical perspective of physical organic chemistry. It is followed by nine plenary lectures, illustrating



The structure of heparin

both old and new trends in physical organic chemistry.

Marie-Françoise Rausse of the University of Paris, France, describes organic reactions in microorganized media. The effect of ion exchanges at the micellar interface in cationic micelles and the electrophilicity of water in reverse micelles are discussed. The chemistry of stable enols is presented by Zvi Rappoport of the Hebrew University, Jerusalem. The detailed pathway of enol formation by the addition of amines to a ketene, mechanism of enantiomerization of chiral triarylenols, and the pK_a values of the enols are discussed.

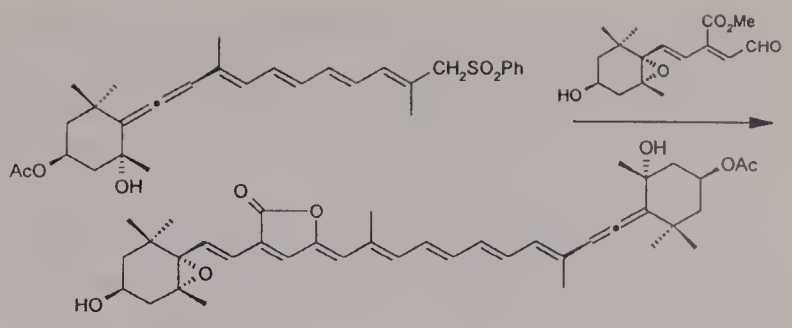
Derek Barton of the Texas A&M University summarizes the use of Gif chemistry in the selective functionalization of saturated hydrocarbon. His lecture illustrates how physical organic concepts can be applied to invent a new organic reaction. Yoshiteru Sakata of Osaka University, Japan, describes the basic principles of how electron transfer can be controlled and utilized to convert solar energy to chemical energy based on model studies, a tool used mostly by physical organic chemists.

Biological science is a new frontier of physical organic chemistry. The thiamin chemistry described by Ronald Kluger of the University of Toronto, Canada, demonstrates how analysis of products, study of reactive intermediates and kinetics can be utilized to understand enzymatic catalysis. The human brain defines a major challenge in all fields of science. Structure–function studies on the nicotinic acetylcholine receptor by Dennis Dougherty of the California Institute of Technology shows that physical organic chemistry can also be applied to the chemistry of the brain.

Three further lectures were developed to supramolecular chemistry. Peter Stang of the University of Utah described self-assembly of molecular squares and rectangles based on square-planar complexes, iodonium species and metallocenes connected by bidentate ligands. Fraser Stoddart of the University of Birmingham, UK, showed that slippage of π-electron deficient bipyridinium-based polyethers through the π-electron rich hydroquinone-based and/or dioxynaphthalene-based macrocyclic polyethers can self-assemble [*n*]rotaxane. Two-dimensional organization of molecules is presented by Toyoki Kunitake of Kyushu University, Japan. He shows that mixed monolayers and multicomponent monolayers can be produced at the air-water interface by utilizing complementary hydrogen bonding.

Carotenoids

The October 1997 issue of *Pure and Applied Chemistry*, **69**(10), contains texts of the main lectures presented at the 11th International Symposium on Carotenoids, held in Leiden, the Netherlands, 18–23 August 1996. A total



Synthesis of peridinin

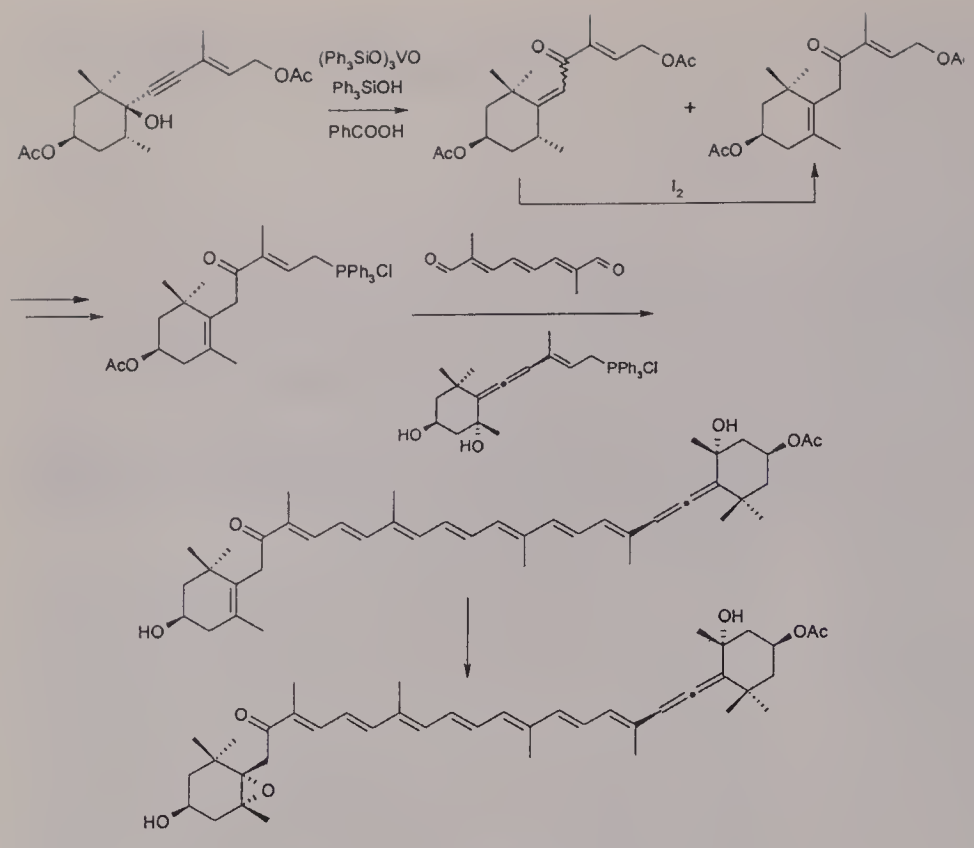
of 21 lectures are published, dealing with aspects ranging from stereochemistry to commercial opportunities for production by biotechnology.

In a preface, Symposium Editor George Britton, of the School of Biological Sciences, University of Liverpool, UK, recalls that the first International Symposium on Carotenoids was held 30 years earlier (1966) in Trondheim, Norway; the expansion and diversification in the carotenoid field is reflected by the fact that, in Leiden, almost ten times as many participants were registered as attended the first meeting. The Leiden Symposium also marked the beginning of a new era for the carotenoid field, with the foundation of a new International Carotenoid Society. The Society will seek to promote carotenoid science and will take responsibility for future International Symposia.

Stereochemical aspects of carotenoids are of importance not just for stereoselective total synthesis and structure elucidation of naturally occurring carotenoids, but also have an impact on biochemical and biological phenomena. Such aspects were dealt with by Synnove Liaanen-Jensen of the Norwegian University of Science and Technology, with examples selected from his own research. Particular emphasis was placed on the interdisciplinary aspects of stereochemistry, and the application of different methods—spectroscopy (VIS, CD, ^{1}H NMR), HPLC, total and partial synthesis, oxidative degradation, derivatization including partial resolution and enzymatic reactions, iodine-catalysed stereomutation and proof of natural occurrence.

Hanspeter Pfander of the University of Berne, Switzerland, presented a progress report on carotenoid synthesis, covering the period 1990–96. This is a continuation of the review given at the 9th International Symposium on Carotenoids held in Kyoto. As 'outstanding achievements' he points to the total synthesis of peridinin and fucoxanthin. Rodney Ausich of Kemin Foods of Des Moines, Iowa, focused on commercial biosynthesis, particularly for carotenoids that cannot easily be synthesized or cannot be produced economically by chemical synthetic techniques. With the new power of biotechnology and recombinant DNA technology, the biosynthetic capability of organisms to produce carotenoids can be enhanced, he says.

A discussion of the role of dietary carotenoids as po-



Synthesis of fucoxanthin

tential cancer preventive agents was provided by John Bertram of the Cancer Research Center of Hawaii. He presents evidence that three major dietary carotenoids, beta-carotene, lutein and lycopene, can increase connexin 43 gene expression in 10T1/2 cells and in human keratinocytes in organotypic culture. He continues to suggest that the conversion of dietary carotenoids to compounds which can increase gap junctional communication may play a role in the protective action of carotenoid-rich foods.

Other lectures included E/Z isomeric carotenes, the fate of carotenoids in sediments, model systems for observing photoreox reactions of carotenoids, photophysics and photochemical properties, carotenoid levels in human lymphocytes, bioavailability of carotenoids, molecular genetics of the carotenoid biosynthesis pathway in plants and algae.

Coordination chemistry

The October issue also contains texts of the six plenary lectures presented at the 31st International Conference on Coordination Chemistry, held at Vancouver, Canada, 18–23 August 1996. The Conference was organized by the Inorganic Chemistry Division in conjunction with the Canadian Society of Chemistry.

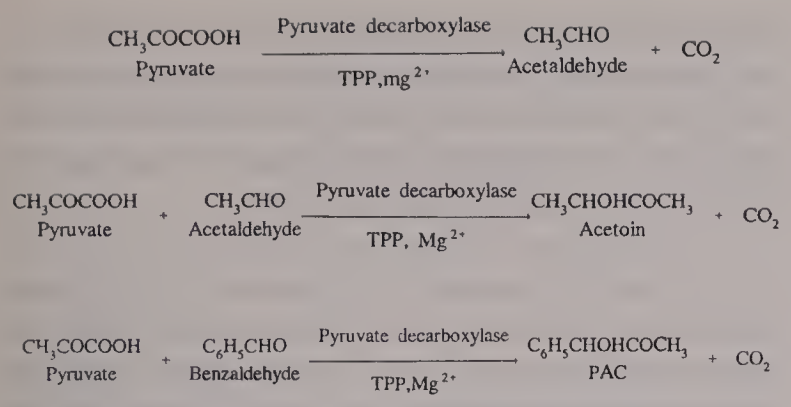
Included is a lecture by Leonard Lindoy of the University of Sydney, New South Wales, on the development of alternate strategies for achieving metal–ion recognition. He considers an important aspect of the research to have been the investigation of metal ion complexation over a range of related macrocycles, incorporating different macrocyclic ring sizes, donor atom set combinations and/or degree of ring substitution and the search for stability maxima at different points in this range. His methodology includes assessment of the possible factors influencing any observed metal-ion recognition behaviour, followed by structural modification of particular ligand systems in an attempt to 'tune up' such behaviour. In particular instances he says it has proved possible to modify a ligand type progressively, using several 'tuning' cycles, such that very considerably enhanced discrimination towards a metal ion of interest has been achieved. In this manner, he says it has also proved possible to elucidate the subtle factors underlying different discrimination mechanisms.

The other five lectures covered: a structural model for silicotungstate monolayers on silver(111); macrocyclic metal complexes for selective recognition of nucleic acid bases and manipulation of gene expression; high oxidation state coordination chemistry with triamidoamine tungsten and molybdenum complexes; X-ray absorption spectroscopic studies of metal centres in biology and developments of relevant synthetic analogues; and coordination chemistry and catalytic conversions of H_2S.

Chemical thermodynamics

The November issue of *Pure and Applied Chemistry*, **69**(11), contains texts of the plenary and invited lectures presented at the 14th International Conference on Chemical Thermodynamics held in Toyonaka, Osaka, Japan, 25–30 August 1996. The Conference was organized by the Physical Chemistry Division in conjunction with the Science Council of Japan, the Chemical Society of Japan, the Japan Society of Calorimetry and Thermal Analysis and the Atomic Energy Society of Japan.

Included is the text of the 11th Rossini Lecture, presented by Robert Alberty of the Massachusetts Institute of Technology. His theme is Legendre transforms, used to introduce intensive variables as natural variables in the fundamental equations of thermodynamics. Prof. Alberty explains that natural variables are important because, when a thermodynamic potential can be determined as a function of its natural variables, all the other thermodynamic properties of the system can be obtained by taking partial derivatives. It is usually more convenient to use thermodynamic potentials that have intensive natural variables because they are often more easily controlled than the conjugate extensive variables. This is illustrated, he says, for chemical reaction systems in which it is of interest to specify the chemical



Production of phenylacetylcarbinol (PAC)

potential of a species (for example, the pH in a biochemical system). Since the electric potentials of phases in a multi-phase system are not natural variables of the Gibbs energy, it is useful to define a transformed Gibbs energy, for which electric potentials of phases are natural variables. The use of Legendre transform brings in a new set of thermodynamic properties, new Maxwell equations, Gibbs–Duhem equations and Gibbs-Helmholtz equations.

Environmental biotechnology

The November issue also contains selected proceedings of an International Conference on Environmental Biotechnology '96 held in Palmerston North, New Zealand, 1–4 September 1996. The published conference papers offer a wide-ranging analysis of the potential of biotechnology to waste treatment, specific perspectives on environmental damage and remediation, industrial research on pollutant mitigation, research into the area of upflow anaerobic sludge blanket reactors, the biological treatment of food industry wastes and two examples of cleaner technology for developments from the pharmaceutical and paper industries.

The cleaner technology examples included production of phenylacetylcarbinol by yeast through productivity improvements and waste minimisation. L-Phenylacetylcarbinol is a precursor for the synthesis of L-ephedrine and D-pseudoephedrine, two pharmaceuticals with nasal decongestant properties. L-Phenylacetylcarbinol is generated biologically through the pyruvate decarboxylase-mediated condensation of added benzaldehyde with acetaldehyde generated metabolically from feed stock sugars via pyruvate. Some of the added benzaldehyde is converted through the action of alcohol dehydrogenase(s) to benzyl alcohol, an undesired by-product. L-Phenylacetylcarbinol extracted from the fermentation broth is converted chemically by hydroamination in the presence of methylamine and hydrogen to L-ephedrine, and then by isomerization to D-pseudoephedrine. Bruce Anderson and colleagues at the Royal Melbourne Institute of Technology present a dual approach strategy to enhance the ratio of product to by-product generated and to minimize the waste treatment burden of the spent fermentation broth. He explains that benzaldehyde delivery to the fermentation has been modified to ensure that sufficient raw material is available, together with pyruvate, during peak periods of pyruvate decarboxylase activity, and that benzaldehyde is less available during periods of high alcohol dehydrogenase activity. The inorganic content of the spent fermentation broth has been reduced substantially by the partial substitution of raw sugar for molasses in the medium, with a reduction of molasses content by 60% resulting in an increase of phenylacetylcarbinol production. Further work on the optimization of the concentration of carbohydrate, nitrogen and phosphate in the fermentation has been conducted and has led, he claims, to further productivity increases, together with reduced waste generation, resulting in an L-phenylacetylcarbinol process which is considerably 'cleaner' than the parent process.

New Publications

Compendium of Chemical Terminology: IUPAC Recommendations, 2nd Edn

Since publication of the first edition in 1987, the IUPAC *Compendium of Chemical Terminology*, popularly referred to as the 'Gold Book' in recognition of the contribution of the late Victor Gold who initiated the work, has been the standard work on chemical terminology. Definitions published by IUPAC are drafted by international committees of experts in the appropriate chemistry subdisciplines and ratified by IUPAC's Interdivisional Committee on Nomenclature and Symbols. In this second edition, the IUPAC-approved definitions are supplemented with some definitions from ISO and from the *International Vocabulary of Basic and General Terms in Metrology*. Since the first edition was published 11 years ago, the majority of the material in the 'Gold Book' has been revised and updated by IUPAC; thus many of the first-edition definitions have been modified or replaced. Furthermore, since 1986 IUPAC has published new terminology documents covering many areas of chemistry not previously treated, and definitions from these documents are now included. Among new areas covered are polymer science, photochemistry, stereochemistry, clinical chemistry, biotechnology, toxicology, class names for organic chemicals and

atmospheric chemistry. The result is a collection of nearly 7000 terms, with authoritative definitions, spanning the whole range of chemistry. All IUPAC recommendations published up to the end of 1995 were considered for inclusion, together with some particularly significant material published in 1996. A selection was made on the basis of general utility; some terms were omitted as being of interest only to a highly specialist audience.

Compendium of Chemical Terminology: IUPAC Recommendations, 2nd edn. Compiled by Alan D. McNaught & Andrew Wilkinson. Published by Blackwell Science, Osney Mead, Oxford OX2 0EL, UK. Price: GBP 39.50/ USD 49.50. ISBN 0-86542-684-8.

Interfacial Science

The ability to design a solid surface with specific properties has been a central theme in research in physical chemistry over the past 20 years. The aims may be as diverse as production of an efficient and selective catalyst and the creation of a new optical device. Over the past decade the emergence of sophisticated surface-sensitive techniques and innovative computational methods has opened up new avenues for exploration in surface science. *Interfacial Science* sees a blurring of the traditional approaches to the condensed phase and surface chemistry, and reflects the broad perspective of the subject. It examines advances and new directions in both experimental and computational approaches and in both fundamental and applied research. Undoubtedly, the book will make an important contribution to one of the most exciting areas of physical chemistry.

Interfacial Science—a Chemistry for the 21st Century monograph. Edited by M.W. Roberts; Foreword by Sir John Meurig Thomas. Published by Blackwell Science, Osney Mead, Oxford OX2 0EL, UK, 1997. ISBN 0-632-04219-2.

Environmental Chemistry in Classroom Experiments

Environmental Chemistry in Classroom Experiments, an English translation of the 1990 German edition of the book *Umweltchemie im Experiment,* is published by IUPAC's Committee on Teaching of Chemistry. The book focuses on the task of teaching environmental chemistry through a hands-on approach by describing 130 close-to-reality experiments. Also described are details of the required equipment, chemicals, procedures, precautions and safety instructions needed for conducting the experiments. This volume is intended as a resource book for teachers of chemistry and biology. The experiments can be integrated in the formal laboratory curricula (for example, as small projects) or used in an informal manner for creating environmental awareness. In addition, several experiments can be used as the basis of classroom demonstrations.

Environmental Chemistry in Classroom Experiments. By Rüdiger Blume and Hans Joachim Bader in collaboration with Manfred Kuballa. Translated by Johannes 'Hans' Bouma. Published for IUPAC Committee on Teaching of Chemistry by S.M.V. Traders and Printers, Delhi 110 009, India, with the permission of Cornelsen Verlag Scriptor, Berlin, Germany. ISBN 81-86968-00-8. Further information can be obtained from Peter Towse, Centre for Studies in Science and Mathematics Education, University of Leeds, Leeds LS2 9JT, UK. Fax: +44 1132 334683. E-mail: p.j.towse@education.leeds.ac.uk

A Proceedings on Cost-Effective Chemistry: Ideas for Hands-on Activities

The proceedings of a workshop hosted by the Institute for Chemical Education at the University of Wisconsin, Madison, 15–26 July 1996, on cost-effective instrumentation and ideas for teaching chemistry are reproduced in the form of a source book. The aim is to stimulate the teaching of chemistry, make the subject more enlightening, and give students a greater experience of hands-on activities. The main topics covered are: low-cost instrumentation; low-cost apparatus; small-scale chemistry and low-cost reagents; chemical and bio-sensors; and low cost microprocessor-based data loggers and instrument controllers.

A Proceedings on Cost-Effective Chemistry: Ideas for Hands-on Activities. Edited by Peter Towse, Centre for Studies in Science and Mathematics Education, University of Leeds, UK, and Amy Huseth, Institute for Chemical Education, University of Wisconsin-Madison, USA. Published on behalf of the Institute for Chemical Education and the International Network for Cost-Effective Science Education by S.M.V. Traders and Printers, Delhi 110 009, India. ISBN 81-86968-01-6.

Macromolecular Symposia, Vol. 118: IUPAC Macro Seoul '96

Volume 118 of *Macromolecular Symposia* presents 96 manuscripts of plenary and invited lectures presented at the 36th International Symposium on Macromolecules held in Seoul, Korea, 4–9 August 1996. The symposium was sponsored by IUPAC, and organized by the Polymer Society of Korea. The volume follows the scientific programme in being divided into a plenary session followed by 11 topic sessions: polymer synthesis and re-

action; polymer structure and properties; thermodynamics and molecular dynamics; polymer processing; polymer blends and composites; polymer membranes; field responsive polymers; biorelated polymers; supramolecular assembly and polymer thin films; polymers and environment; and polymer education.

Macromolecular Science, Vol. 118: IUPAC Macro Seoul '96. Symposium Editor, Jung-Il Jin; Editor-in-Chief, Hartwig Höcker; Editors, R.E. Bareiss, W. Guth, B. Jung & I. Meisel. Published by Hüthig & Wepf Verlag, Zug, June 1997, pp 1–766. ISSN 1022-1360. Price (Vol. 118): Sfr 246/DM 290/USD 176, plus mailing.

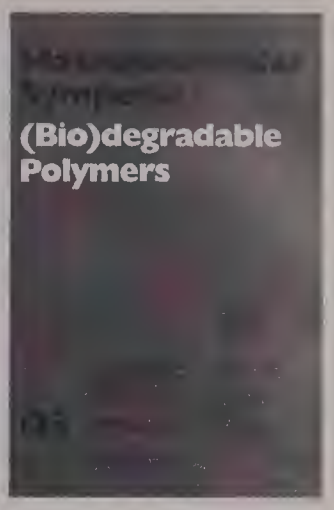
Macromolecular Symposia, Vol. 122: Polycondensation

Volume 122 of *Macromolecular Symposia* presents invited lectures and selected contributions presented at the International Symposium of Polycondensation, Related Processes and Materials held in Paris, France, 23–26 September 1996. The symposium was sponsored by IUPAC in conjunction with the European Polymer Federation, Centre National de Recherche Scientifique, GFP—Division Polymères et Elastomères de La Société Française de Chimie and the Université Pierre et Marie Curie—Paris, and was held in honour of Prof. Ernest Maréchal.

Macromolecular Science, Vol. 122: Polycondensation. Symposium Editor, Alain Fradet; Editor-in-Chief, Hartwig Höcker; Editors, W. Guth, B. Jung, I. Meisel & S. Spiegel. Published by Hüthig & Wepf Verlag, Zug, August 1997, pp. 1–386. ISSN 1022-1360. Price (Vol. 122): Sfr 140/DM 164/USD 99, plus mailing.

Macromolecular Symposia, Vol. 123: (Bio)degradable Polymers

Volume 123 of *Macromolecular Symposia* presents most of the invited main and special lectures presented at the 37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects held in Prague, the Czech Republic, 15–18 July 1996. The symposium was sponsored by the Macromolecular Division of IUPAC in conjunction with the Academy of Science of the Czech Republic and the Czech Chemical Society.



Macromolecular Science, Vol. 123: (Bio)degradable Polymers. Symposium Editor, J. Kahovec; Editor-in-chief, Hartwig Höcker; Editors, W. Guth, B. Jung, I. Meisel & S. Spiegel. Published by Hüthig & Wepf Verlag, Zug, September 1997, pp. 249. ISSN 1022-1360. Price (Vol. 123): Sfr 90/DM 106/USD 65, plus mailing.

Sustainability Indicators: Report of the Project on Indicators of Sustainable Development

To be able to track progress towards the Agenda 21 'sustainable development' blueprint passed at the UN Conference on Environment and Development held in Rio in 1992, scientists have been required to devise measuring sticks, or sustainable development indicators, showing where we are and which way we are headed. Such indicators serve both as an information tool and as the basis for policy making. SCOPE, the Scientific Committee on Problems of the Environment, has collected and coordinated work on sustainability indicators from around the world, and the results are presented in this book. Included are a rich diversity of perspectives and approaches, described by more than 50 contributors from many different countries and cultures working in a wide range of fields and organizations at all levels.

Sustainability Indicators: Report of the Project on Indicators of Sustainable Development. Edited by Bedrich Moldan & Suzanne Billharz. Published by John Wiley & Sons, Baffins Lane, Chichester, West Sussex PO19 1UD, UK, 1997. ISBN 0-471-97352-1.

Conferences

12th International Conference on Organic Synthesis, Venice, Italy, 28 June–2 July 1998

The conference will deal with all important aspects of modern organic synthesis. The scientific programme will consist of:

- ten plenary lectures (60 minutes including discussion) and a Thieme IUPAC prize lecture
- six lectures (30 minutes including discussion) in a mini symposium on combinatorial chemistry in drug

discovery

- 36 section lectures (30 minutes including discussion) in four parallel sessions on the following topics: new synthetic methods; stereoselective synthesis; metal-mediated synthesis; and target oriented synthesis
- oral communications (15 minutes including discussion) in four parallel sessions on the same topics as the section lectures
- poster sessions

Participants wishing to present a poster must send a completed Abstract Form, along with two photocopies to the Organizing Secretariat by 15 January 1998.

The registration fee for participants is Lira 900 000 before 1 April 1998, Lira 1050 000 after 1 April 1998, and for students Lira 450 000 before 1 April 1998 and Lira 550 000 after 1 April 1998. The registration fee includes admission to the scientific sessions, conference kit (final programme, abstract book), coffee/tea during the official breaks, pack lunches, welcome cocktail on Sunday 28 June and concert on Tuesday 30 June.

For further information, please contact: The Organizing Secretariat, ICOS-12, Depha Congress, Via Cassanese 224, Palazzo Tiepolo, 20090 Segrate (MI), Italy. Tel.: +39 2 21 69 121. Fax: +39 2 26 92 91 63. E-mail: dephadue@mbox.vol.it

15th International Conference on Chemical Education: Chemistry and Global Environmental Change, Cairo International Conference Center, Ain Shams University, Cairo, Egypt, 9–14 August 1998

This conference, organized by the Department of Chemistry, Faculty of Science, Ain Shams University, is the first International Conference on Chemical Education (ICCE) event to be held in Africa and in the Arab States. The conference theme—Chemistry and Global Environmental Change—conforms with Chapter 36 of Agenda 21 of the Rio declaration of the UN Conference (in Brazil—1992) on Environment & Development which is concerned with 'promoting education, public awareness and training'.

The technical programme of the 15th ICCE conference will be developed around the leading role of chemistry in reducing the growing harmful effects on the environment. The need to increase environmental literacy by encouraging environmental chemistry instruction as an important part of general education at all levels (elementary school through university) is of great concern to all educators.

Speakers will include chemistry Nobel Laureates, eminent chemists and chemistry educators of international renown. Many of the presentations will enlarge on the conference theme, chemistry research, and chemistry education into the 21st century. Additional highlights include an exhibition programme, which will provide an opportunity to observe the most recent developments and application of contemporary environmental techniques. The conference will also feature plenary lectures, symposia, presentations, workshops and poster sessions. Chemists and chemistry educators will have a unique opportunity to discuss and share their work.

In addition, socio-cultural and guest programmes are being planned which will introduce the ancient and present Egyptian way of life and the history of Pharaonic, Roman, Coptic and Islamic Egypt.

A second circular will be distributed in December 1997.

The registration fee will be approximately USD 350 per person including the conference lunches, morning and afternoon teas, abstract book, some social events, receptions and transportation from the hotels to the conference centre. IUPAC Affiliate Members will receive a 10% reduction.

For further information, please contact: Prof. Saad S.M. Hassan, Chairman of the Organizing Committee of 15th ICCE, Department of Chemistry, Faculty of Science, Ain Shams University, Cairo, Egypt. Tel./Fax: +20 4831836 – 2842123. Telex: 74070 USMMS. E-mail: iupac15@asunet.shams.eun.eg

37th IUPAC Congress—Frontiers in Chemistry: Molecular Basis of the Life Sciences, International Congress Center, Berlin, Germany, 14–19 August 1999

The title does not mean a Congress solely concentrating on Biochemistry or Molecular Biology. On the contrary, IUPAC invites scientists from all fields of chemistry and from all over the world to demonstrate the importance of all fields of synthetic, analytical and theoretical chemistry to the subject. The scope of the parallel 27th General Meeting of the German Chemical Society will be much broader and will highlight the current state

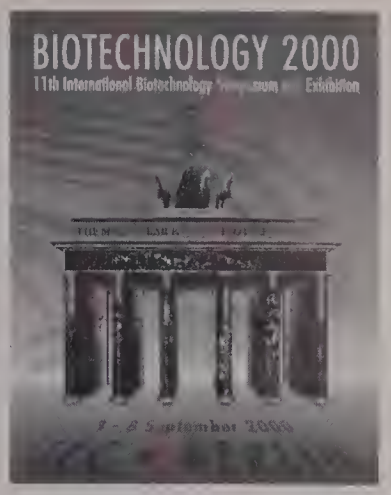
of research in the Federal Republic of Germany.

Both organizations would like to invite you to participate at this exciting event, which promises to become one of the largest and most fascinating chemistry conventions world-wide at the end of the 20th century.

For further information, please contact: Prof. Heindirck tom Dieck, Gesellschaft Deutscher Chemiker, IUPAC/ GDCh 99, PO Box 90 04 40, D-60444 Frankfurt-am-Main, Germany. Tel.: +49 69 7917 358, 360 or 366. Fax: +49 69 7917 475. E-mail: tg@gdch.de.

11th International Biotechnology Symposium and Exhibition: Biotechnology 2000, International Congress Center, Berlin, Germany, 3–8 September 2000

The International Biotechnology Symposia (IBS), held every four years, are the leading world-wide meetings in the field of biotechnology. The title 'The Molecular Key for Biotechnology' has been chosen for this International Biotechnology symposium because of the rapid development of biotechnology in conjunction with results in fundamental biological sciences. This theme will characterize the world in the next millennium, which to a large extent will use molecular biology and genetic engineering for the benefit of mankind.



As at previous IBS meetings, the scientific programme will be composed of a number of symposia, workshops, poster presentations and an exhibition. Round tables will be organized to discuss controversial scientific and ethical problems with a larger audience. The aim of the Symposium is to review the present state-of-the-art, to discuss the way in which pure and applied research in different fields of science and technology interact, and to demonstrate the interdisciplinary nature of biotechnology.

An Exhibition will be organized in conjunction with the Symposium.

If you wish to present a paper/poster or to exhibit please contact: Dechema eV, c/o 11th IBS, Theodor-Heuss-Allee 25, D-60486 Frankfurt am Main, Germany. Tel.: +4969 7564 241. Fax: +49 69 7564 201. E-mail: info@dechema.de

Conference Calendar

1997

Biodiversity and bioresources

23–27 November
International Conference on Biodiversity and Bioresources—Conservation and Utilization. Phuket, Thailand.
IUPAC Biodiversity Conference, National Center for Genetic Engineering and Biotechnology, National Science and Technology Development Agency Building, 73/1 Rama VI Road, Bangkok 10400, Thailand. Tel.: +66 (2) 6448150-4, ext. 505, 532, 534; Fax: +66 (2) 6448107-8; E-mail: iupacconf@biotec.or.th

1998

Polymer sciences and technology

5–10 January
International Symposium on Advances of Polymer Sciences and Technology. Madras, India.
Dr K.S.V. Srinivasan, Deputy Director & Head, Polymer Division, Central Leather Institute, Council of Scientific & Industrial Research, Adyer, Madras - 600 020, India.

Calorimetry and chemical thermodynamics

5–9 April
International Conference on Calorimetry and Chemical Thermodynamics. Campinas, Brazil.
Prof. C. Airoldi, Instituto de Química, UNICAMP - CP 6154, Universidade Estradul de Campinas, 13081-970 Campinas sp, Brazil.
http://www.iqm.unicamp.br/wloh/conf/

Trace element speciation

4–7 May
1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences. Neuherberg, Munich, Germany.
First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, FRG. Tel.: +49 (89)

31873030 (2669); Fax: +49 (89) 31873362.

Degradation processes in the environment

24–28 May
International Conference on Degradation Processes in the Environment. Dubrovnik, Croatia.
Dr A. Sabljic, Institute Boskovic, POB 1016, HR-10011 Zagreb, Croatia

Organic synthesis

28 June–2 July
12th International Conference on Organic Synthesis. Venice, Italy.
Depha Congress SRL, Viale Majno 21, 20122 Milano, Italy. Tel.: +39 (2) 76008190; Fax: +39 (2) 782400; E-mail: dephadue@mbox.vol.it

Chemistry in Africa

6–10 July
7th International Chemistry Conference in Africa (7th ICCA). Durban, South Africa.
The Secretary, 7th ICC & 34th SACI Convention, Department of Chemistry & Applied Chemistry, University of Natal, Durban 4041, South Africa. Tel.: +27 (31) 3603090. Fax: +27 (31) 2603091; E-mail: 7icca@che.und.ac.za

Macromolecules

13–17July
37th International Conference on Macromolecules, Gold Coast, Australia.
Prof. R.G. Gilbert, School of Chemistry, F11, Sydney University Polymer Center, University of Sydney, New South Wales 20006, Australia. Tel.: +61 (2) 351 3366; Fax: +61 (2) 351 3329;
E-mail: gilbert@chem.usyd.edu.au

20–23 July
18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.
P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, CZ-162 06 Prague 6, Czech Republic. Tel.: +420 (2) 360341; Fax: +420 (2) 367981;
E-mail: sympo@imc.cas.cz

Chemical thermodynamics

26 July–1 August
15th International Conference on Chemical Thermodynamics. Porto, Portugal.
Prof. M.A.V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal.

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (171) 4378656; Fax: +44 (171) 7341227.

Novel aromatic compounds

2–7 August
9th International Symposium on Novel Aromatic Compounds, Hong Kong.
Prof. H.N.C. Wong, Chairman, Local Organizing Committe, 9th International Symposium on Novel Aromatic Compounds, Department of Chemistry, Chinese University of Hong Kong, Shatin, New Territories, Hong Kong.

Solubility phenomena

5–8 August
8th International Symposium on Solubility Phenomena. Niigata, Japan.
Prof. H. Akaiwa, Faculty of Engineering, Gunma University, Kiryu 376, Japan.

Chemical education

9–14 August
15th International Conference on Chemical Education: Chemistry and Global Environmental Change. Cairo, Egypt.
Prof. Saad S.M. Hassan, Department of Chemistry, Faculty of Science, Ain Shams University, Cairo, Egypt.

Physical organic chemistry

16–21 August
14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.
Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento di Química, 88040-900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy. Tel.: +39 (55) 2757549. Fax: +39 (55) 2757555.

Medicinal chemistry

6–10 September
25th International Symposium on Medicinal Chemistry. Edinburgh, Scotland.
Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (0)171 437 8656; Fax: +44 (0)171 734 1227.

Natural products

11–16 October
21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.
Prof. Xibai Qiu, Secretariat of ISCNP-21, c/o Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: +86 (10)

62568157 or 62564020; Fax: +86 (10) 62568157; E-mail: qiuxb@infoc.3.icas.ac.cn

1999

IUPAC General Assembly

7–14 August
40th General Assembly. Freie University of Berlin, Berlin, Germany.

The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion.

IUPAC Congress

14–19 August
37th IUPAC Congress. International Congress Center, Berlin, Germany.
Prof. Heindirck tom Dieck, Gesellschaft Deutscher Chemiker, IUPAC/GDCh 99, PO Box 90 04 40, D-60444 Frankfurt-am-Main, Germany. Tel.: +49 69 7917 358, 360 or 366. Fax: +49 69 7917 475. E-mail: tg@gdch.de

2000

Macromolecules

9–14 July
MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.
Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90-363 Lodz, Poland. Tel.: +48 (42) 819815; Fax: +48 (42) 847126.

Biotechnology

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.

How to apply for IUPAC sponsorship

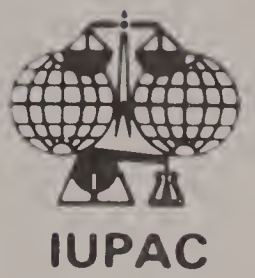
To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* 1992, **14**, 203.

Index

ACS/IUPAC/CMA/EPA Collaborative Symposium 129
Air Pollution Profile of Turkey 190
Appointment of new Executive Director 65
Atmospheric chemistry, measurement technologies in 170
Biochemical Nomenclature, IUPAC–IUBMB Joint Commission on 116
Biophysical Chemistry, Introduction to Commission on 113
Chemical MIME Project 17
Chemical Society Presidents, Meeting of 183
The Chemist, Facing the Structural Changes in the Chemical Industry 183
CHEMRAWN IX, Conference Report 127
CHEMRAWN in Montevideo 171
Colleagues Deceased 51, 69, 172, 193
Comments
  An editor's lot... 141
  The antiscience cancer 142
Commission News
  Biotechnology 194
  Chemical Kinetics (I.4) 193
  High Temperature Materials and Solid State Chemistry (II.3) 70
  Physical Organic Chemistry (III.2) 70
  Soil and Water Chemistry 195
  Subcommittee on Transport Properties 193
Conference Calendar 35, 60, 90, 146, 174, 227
Conferences 31, 59, 86, 145, 173, 225
Contaminants in Soil, Fate and Effects of 136
COSPAR scientific assembly 171
Crystal Growth Awards 68
Election of Officers and Bureau Members 97
Endocrine Disrupters, 'White Book' on 191
Fate and Effects of Contaminants in Soils 136
Federation of European Chemical Societies, General Assembly 49
Green Chemistry: Challenging Perspectives, International Conference on 187
Human genomics conferences, IFFC/Roche establish 172
International Council for Chemistry 67
International Council of Scientific Unions, new Executive Director 192
International Newsletter on Chemical Education 192
International Organization for Chemical Sciences in Development (IOCD) 12
IUPAC
  Access to Documents on the WWW 30
  Accounts for 1996 108
  Biennial Report of the Treasurer and Finance Committee 158
  Future Directions, Meeting on 66
  Joint Commission with IUBMB on Biochemical Nomenclature 116
  President's Report 152
  Relocation of Archival Material 161, 191
  Relocation of Secretariat 94, 151
  Secretary General's Report 156
  Treasurer's Review 1991–1997 160
  1996 Report 104
  36th Congress 1, 180
  39th General Assembly 1, 96, 177
Jost, John, Appointment of new Executive Director 65
Letters to the Editor 57, 143
Maison de la Chimie Foundation Prize 24
Measurement technologies in atmospheric chemistry 170
Mycotoxins and Phycotoxins, IXth International IUPAC Symposium 24
Names and Addresses 24, 52, 69, 126, 172
PAC Reviews 41, 72, 169, 220
Pesticide Residues in Food, Safety Evaluation of 119
Photochemistry in Italy 7
Polish Chemical Industry, Training for 20
Provisional Recommendations
  Analytical aspects of chemically modified electrodes 196
  Definition of terms relating to the non-ultimate mechanical properties of polymers 58
  Extension and revision of the von Baeyer system for naming polycyclic compounds 196

Extension and revision of the nomenclature for spiro compounds 196
Glossary of terms used in medicinal chemistry 82
Names for inorganic radicals 140
Nomenclature of glycolipids 58
Nomenclature, symbols, units and their usage in spectrochemical analysis XIV 59
Parameters and symbols for use in nuclear magnetic resonance 58
Recommendations for the presentation of NMR structures of proteins and nucleic acids 140
Revised section F: Natural products and related compounds 82
Publications
Compendium of Chemical Terminology: IUPAC Recommendations, 2nd Edition 223
Environmental Chemistry in Classroom Experiments 224
Fundamental Toxicology for Chemists 54
Hrvatska Nomenklatura Anorganske Kemije 56
Interfacial Science 224
IPCS Health and Safety Guides 80
IUPAC Solubility Data Series, Volumes 63–65 79
Kemisk Ordbog 144
Laboratory Diagnosis of Group A Streptococcal Infections 81
Macromolecular Symposia
(Bio)degradable Polymers 225
Macro Seoul '96 224
Polycondensation 225
Medicinal Chemistry: Today and Tomorrow 79
Molecular Electronics—a 'Chemistry for the 21st Century' monograph 173
Nomenklatura Chromatograficzna 144
Nomenklatur der Organischen Chemie: Eine Einführung 80
Particle Flux in the Ocean 56
A Proceedings on Cost-Effective Chemistry 224
SCOPE Publications
Functional Roles of Biodiversity: A Global Perspective 81
Global Change: Effects on Coniferous Forests and Grasslands 81
The Work of Nature: How the Diversity of Life Sustains Us 80
Sustainability Indicators 225
Use of Recovery Factors in Trace Analysis 80
World Health Organization Publications—Environment 145
Reactivity of Solids: Past, Present and Future 26
Recent Reports
Analytical chiral separation methods 213
Analytical methodology for the determination of aluminium fractions in natural fresh waters 22
Atomic weights of the elements 1995 77
Basic terminology of stereochemistry 75
Biotransformation of non-natural compounds 216
Calculation and application of coverage intervals for biological reference values 215
Characterization of finite length composites: Introduction 217
Characterization of finite length composites: Mechanical performance 218
Characterization of finite length composites: Modelling of stiffness 218
Characterization of finite length composites: Studies on thin sections 218
Characterization of SiC powders and the influence of powder properties on sintering 166
Chemically modified electrodes: Recommended terminology and definitions 167
Chirality in synthetic agrochemicals: Bioactivity and safety consideration 167
Classification and characterization of stationary phases for liquid chromatography: Part I. Descriptive terminology 214
Classification and characterization of stationary phases for liquid chromatography: Part II. Ion exchange 214
Collaborative study of the structure and rheological properties of EVOH/SMA blends 23
Consistency of pH standard values with the corresponding thermodynamic acid dissociation constants 167
Critical evaluation of the use and analysis of stable isotopes 219
Critically evaluated propagation rate coefficients in free radical polymerizations 22
Definitions of terms relating to degradation, aging, and related chemical transformations of polymers 76
Determination of *trans* unsaturated fatty acids in edible oils and fats 219
General features of contracts for natural product collaborations 77
Glossary of basic terms in polymer science 76
Glossary of terms used in bioinorganic chemistry 166
Glossary of terms used in computational drug design 165
Glossary of terms used in photochemistry 76
Guidelines for publication of equations of state. I: Pure fluids 166
Importance of natural organic material for environmental processes in waters and soils 215
Intrinsic characterization of continuous carbon fibre thermoplastic composites 166
Laser-based molecular spectroscopy for chemical analysis—luminescence 213
Laser-based molecular spectroscopy for chemical analysis—Raman scattering processes 213
Measurement and interpretation of complexation phenomena in seawater 22
Methods for the analysis of transient absorbance data 163
Molecular characterization of commercial polypropylene 164
Molecular spectroscopy: General spectroscopic notation 216
Molecular spectroscopy: Permutation and permutation–inversion symmetry notation 216
Molecular spectroscopy: Symmetry notation 216
Nomenclature of carbohydrates 52
Nomenclature of inorganic chains and ring compounds 217
Nomenclature for non-linear chromatography 22
Nomenclature and terminology of fullerenes 213
Optimum use of available residue data in the estimation of dietary intake of pesticides 168
Pesticide fate in tropical soils 168
Preservation and utilization of natural biodiversity 77
Properties and units in the clinical laboratory sciences:
kinds of property 164
properties and units in thrombosis and haemostasis 165
Quantitative analysis of a $PbO–SiO_2$ glass by electron microprobe 23
Reference Value Standards and Primary Standards for pH measurements 164
Reporting of relative sulfur isotope-ratio data 78
Stability constants for alpha-hydroxycarboxylic acid complexes with protons and metal ions 78
Stability constants of complexes of thiocyanate ion 214
Stability constants of metal-imidazole and metal-histamine systems 215
Statistical overview of procedures for determining the limits of detection and quantification 78
Terminology for membranes and membrane processes 21
Relocation of IUPAC Secretariat 94
Retirement of Mo Williams 65
Safety Evaluation of Pesticide Residues in Food 119
Science International: A History of the International Council of Scientific Unions 29
Secretary General's Column 6, 95, 177
Spectroscopic Data Standards, Working Party on 39
Sustainable Environment: National and International Perspectives, a Conference Report 83
Training for the Polish Chemical Industry 20
Transfermium Elements, IUPAC Proposes Names for 68
Turkey, Air Pollution Profile of 190
'White Book' on Endocrine Disrupters 191
Williams, Mo, Presentation to 179
Williams, Mo, Retirement of 65
Working Party on Spectroscopic Data Standards 39
World Science Report 1996 14
World Wide Web, Use of for Access to IUPAC Documents 30

International Union of Pure and Applied Chemistry (IUPAC)



President: A. E. FISCHLI (*Switzerland*)
Vice-President: J. JORTNER (*Israel*)
Secretary-General: E. D. BECKER (*USA*)
Treasurer: J. M. WARD (*UK*)

IUPAC Secretariat

PO Box 13757, Research Triangle Park, NC 27709-3757, USA. Tel.: +1 (919) 485 8700. Fax +1 (919) 485 8706. E-mail: johnwjost@compuserve.com

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification
- to co-operate with other international organizations which deal with topics of a chemical nature
- to contribute to the advancement of pure and applied chemistry in all its aspects

The membership of IUPAC presently comprises 39 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Neue Schweizerisches Chemische Gesellschaft **(Switzerland)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1997, Vol. 19, No. 6 (November)

177 Secretary General's Column
Edwin D. Becker

179 Presentation to Dr Mo Williams

180 36th IUPAC Congress

183 Meeting of Chemical Society Presidents

187 Conference Report

190 Air Pollution Profile of Turkey

191 News

193 Commission News

196 Provisional Recommendations

197 Names and Addresses of Officers of IUPAC bodies 1998–99

213 Recent Reports

220 PAC Review

223 New Publications

225 Conferences

227 Conference Calendar

229 Index

Information on this magazine can be accessed at http://www.blackwell-science.com/products/journals/chem.htm

Blackwell Science

0193-6484(199711)19:6;1-A

Printed in Great Britain by Alden, Oxford, Didcot & Northampton